RZWQM-Sed Project Final Report

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Executive Summary

Sediment runoff is one of the important processes contributing to pesticide offsite movement. However, few of the field scale agricultural models that currently exist can track farm processes, plant growth kinetics, nutrient cycling, reactive chemistry of applied non-fertilizer chemicals, hydrologic flow through the vadose zone and across the surface, and sediment runoff with the possibility of sorbed chemicals. Those that do are usually weak in one or more of the above required capabilities For the California Department of Pesticide Regulation, this is a serious deficit in the modeling toolboxes of project scientists, regulators, and decision makers. To address this need, the ultimate goal of this project is to identify compatible existing models which can account for these factors, and then integrate them into a single model which can accurately predict sediment-bound pesticide offsite movements.

Among existing agricultural models, the Root Zone Water Quality Model (RZWQM) is one of the better candidates for simulating pesticide runoff under California's agricultural conditions. RZWQM is a mechanistic model, initially developed by the United States Department of Agriculture's Agricultural Research Services (USDA ARS)[1]. It is designed to simulate plant growth and the movement of water, nutrients and pesticides in an agricultural system. The model has been widely used around the world to simulate water and agrochemical movement as impacted by different management practices. The pesticide sub-model includes detailed algorithms for simulating pesticide transport and fate in 4 compartments: crop foliage, crop residues, soil surface and soil sub-surface or root zone.

However, RZWQM lacks the crucial sediment runoff component. This is a significant limitation since both bulk sediment runoff and pesticides sorbed to sediment particles are major components of non-point source pollution. To overcome this limitation, two related, yet distinct, sediment models were integrated into RZWQM: the sediment and surface flow components of both the Groundwater Loading Effects of Agricultural Management Systems (GLEAMS) model and the Water Erosion Prediction Project (WEPP) model.

The integrated model (RZWQM-Sed) was then assessed for accuracy by calibrating and validating using several real world datasets which span a range of spatial and temporal scales: a very small scale bare soil plot, a multi-year field trial of alfalfa run by DPR, a multi-decade watershed scale corn field, and a multi-year olive orchard trial. These trials span space (6 m^2 to 30 ha), time (60 min to 32 years), slope (0.14% to 15%), and plant types (bare soil, uniform coverage, trees). Applying the model to such varied field trials can reveal the circumstances under which it yields either reliable or unreliable predictions. For example, RZWQM was unable to calculate any water runoff (and, therefore, no sediment runoff) with the soil parameters and water input of the bare soil trial data (Colorado Agricultural Research Development & Education Center experimental (ARDEC) site).

After the model RZWQM-Sed integration, a sensitivity analysis was completed to ascertain which variables, especially those variables that cannot be measured in the field, have the greatest influence on both surface water flow (the primary driver of sediment runoff) and sediment concentration in the runoff water. A Morris one-at-a-time and a Sobol variational sensitivity

analyses were performed on RZWQM-Sed, focusing on variables affecting water runoff and sediment yield.

The sensitivity analysis indicated that the precipitation intensity calculated by RZWQM was not compatible with WEPP's internal governing equations. This resulted in predictions of sediment flow that were several magnitudes lower than measured. Dr. Jim Ascough from the USDA ARS is currently looking into the source of the conflict and might be able to rectify it. Until then, WEPP was dropped from further analysis, and only GLEAMS sediment routines were used for calibration and validation.

This report includes the results from the sensitivity analysis and calibration/validation of the GLEAMS-RZWQM integration and further avenues for study. It also includes the unsuccessful results from the WEPP integration and modeling of the data from the bare soil experimental site, since the problems discovered are worth noting.

The highlighted results are as follows.

- Most sensitive water runoff parameters in RZWQM: residual and saturated water content and Brooks-Corey bubbling pressure
- Most sensitive sedimentation parameters in GLEAMS: Universal Soil Loss Equation factors and Manning's N
- RZWQM-Sed prediction of water runoff (Nash-Sutcliffe values range over [-1,1] with 1 being perfect match, 0 indicating that the predictions are as accurate as the mean of the observed data, and <0 indicating predictions less accurate than the mean of the data):
    - For field sized areas at a sub-daily time step, predicted runoff was statistically worse than simply taking the average of previous measurements (Olive orchard Nash-Sutcliffe = -0.49).
    - For watershed sized areas calibrated to yearly summations, predicted runoff was worse than using an average of previous measurements (Treynor Nash-Sutcliffe = -0.27).
    - There was minimal change in predicted runoff when irrigation varied within realistic bounds. The predicted range of runoff amounts was much less than the measured range (ex Treynor data - Measured: average = 16.9, standard deviation = 8.4; Modeled: average = 15.3, standard deviation = 3.1).
- RZWQM-Sed prediction of sediment runoff:
    - Followed the water runoff predictions
    - Often no better than using a past average (Treynor Nash-Stucliffe = 0.032; CDPR alfalfa Nash-Sutcliffe = -0.104)
    - Better in predicting field scale results than watershed scale (Treynor average absolute percent error = 2211; CDPR alfalfa average absolute percent error = 154)
    - Less variation in predicted output compared to the range of measured output or water input.
- Prediction of sediment sorbed pesticide mass in the outflow accurately tracked measured values without any calibration of the pesticide variables. The greatest difference between predicted and measured pesticide mass was that the predicted values had a longer tail of detection leading to conservative estimates of mass flowing off field. Calibration of pesticide variables can eliminate this discrepancy.

The implications of these findings:

- RZWQM-Sed is an excellent model for predicting sediment sorbed pesticide mass in the tailwater under various best management practice regimes.
- RZWQM-Sed is statistically not much better than using an average of past measurements for predicting water and soil mass runoff (see Nash-Sutcliffe statistics above). While not ideal, this still means that comparisons can be made between different management practices to determine which produces the least amount of sediment runoff given changes in cropping, irrigation, soil content, and presence or absence of a cover crop. End users of the model have found the predicted runoff results to be better than most available field scale models and that the accuracy of the model is acceptable for the kind of tasks it will be used for.
- RZWQM-Sed is best used for modeling cases of field sized, uniform cropland, in timeframes spanning a single runoff event to a few years. Modeling heterogeneous regions, large areas, or multi-decade time scales is not recommended.

The performance of the integrated RZWQM-Sed could be further improved. A fundamental problem is that, by design, neither RZWQM nor GLEAMS allow for much complexity in the system. Both models transform the continuous complexity of reality into extremely simplified numerical models. In addition to simplifying 3D space into two 1D flow lines, both models also limit the number of computational cells that can have distinct values to double digits or less. This limitation was necessary several decades ago when the models were initially developed and available computation power was much more limited than it is today. Even the low-end desktop computers available today have the computational power to handle multiple dimensional data and orders of magnitude more cells than RZWQM and GLEAMS use.

An ideal agriculturally-focused environmental model would allow for modeling in two or three dimensions. It should track water, sediment and solutes in the plant canopy, across the soil surface, and through the vadose zone. It should be able to model plant growth and the plant's interaction with applied water and chemicals. It should be easy to expand and extend. It shouldn't depend on proprietary software to compile or run.

Such a model could be built from currently available technology, with less effort than attempting to modify either RZWQM or GLEAMS to model more dimensions, more cells, or more physically-based governing equations. Current open source photogrammetry tools can build a 3D mesh of an actual farm field using a collection of digital photographs. Available finite element modeling tools can be used to build a model from an arbitrary selection of interrelated partial differential equations covering water and soil movement, reactive chemistry, plant growth, nutrient cycling, and any other processes of interest. Current plant geometry modeling tools can be used to derive a very realistic canopy and root zone, which can then be used as inputs to the governing partial differential equations. The end result would be a highly detailed, extendable, physical model that represented reality at a far finer resolution than is available in current models. This would in turn allow for incorporating the heterogeneity that is beyond the capability of all current models.

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Appendix A: Completed tasks done in this project

1. Updated RZWQM codebase to compile under Microsoft Visual Studio using Intel Fortran. Many small errors in variable declarations and formatting needed to be fixed for successful compilation under the stricter Intel Fortran compiler. A version was also ported to GNU's Fortran compiler, which required a more extensive level of code modification, including the use of the automated code rewriting tool plusFORT. There was minimal interest amongst the ARS group for a multi-platform port, so work was halted after a baseline clean compile had been completed. The remainder of development was done on Visual Studio with Intel Fortran.

2. Integrated GLEAMS daily sediment runoff model into RZWQM. If a GLEAMS specific input file is present, it is read and the GLEAMS erosion module is called at each daily time step in which RZWQM determined that runoff had occurred. New code was added to RZWQM to read the input files into global variables and initialize other variables (e.g., soil texture and field size) using RZWQM's internal state. New output code was also written to produce a condensed, easy-to-parse sediment flow output file which lists the following for all days with surface runoff: surface runoff amount, bulk sediment loss, and concentrations of sediments of various size classes in the tail water. A second output file lists the mass of each pesticide modeled that flowed offsite along with the sediment.

3. Integrated the WEPP-Standalone sediment runoff model into RZWQM. Jim Ascough and ARS supplied a cleaned, modularized version of the WEPP sediment model which was then inserted into RZWQM alongside the GLEAMS model. Initial debugging revealed several minor corrections necessary for the WEPP codebase to support repeated calling without modifying the input variables. Testing revealed that the supplied model was producing results orders of magnitude out of range so work was done in collaboration with Jim Ascough to fix the WEPP code. As with the GLEAMS integration, additional input and output code was written in order to read the parameters from an input text file and output the results in an easily parsable plain text format.

4. Created sample input files to model Phil Heilman's basin level dataset, Jim Ascough's ARDEC experiment, Spanish olive orchard, and DPR's alfalfa field experiments; all calibrated to match measured outputs. Each dataset was used to test certain aspects of the model and as base for the automated parameter study. Phil Heilman's dataset is a large scale watershed model that covers many hectares and spans several decades. GLEAMS and WEPP were designed for this type of large scale spatial and temporal averaging, but RZWQM was desgined for a smaller space and time. DPR's alfalfa models cover a single field for just over two growing seasons and employ RZWQM's irrigation, fertilization, crop growth, and pesticide subroutines. The ARDEC dataset covers a very small, unvegetated plot of land for only 1-3 storm events. It is ideal model for testing just the added sediment components and RZWQM's surface runoff calculations.

5. Ran a sensitivity analysis on RZWQM and the GLEAMS component, studying parameter sensitivity to both surface runoff and sediment load. Each sensitivity analysis experiment required 10,000s of model runs over the entire parameter space. In addition to indicating which parameters need to be most carefully considered, these mass model runs also tested the stability of the model and subcomponents, and revealed errors which were fixed. DATKOTA, from Sandia National Labs, was used for the batch model runs.

Input parameter selection and output analysis was accomplished using custom Python codes that utilized Sobol sampling and statistical analysis. A similar sensitivity analysis was done for the WEPP sub-model: while the influential parameters were discovered, the range of values for sediment flow was several orders of magnitude less than it should be. This led to the dropping of WEPP from the final integrated model.

6. Drafted a paper discussing the sensitivity analysis of RZWQM, and GLEAMS, and WEPP with respect to surface flow and sediment loading. Sensitivity analysis for both a vegetated model (based on DPR's alfalfa experiment) and a bare soil model (based off the ARDEC experiment) were completed for all variables in RZWQM related to infiltration and runoff and all sediment specific variables in GLEAMS and WEPP. Both Morris one-at-a-time and Sobol variation analysis methods were used to quantify the influence of all variables on surface flow and sediment run off. The paper is currently being prepared for submission for publication.

7. Drafted a user manual for the new sediment subsystems. Documentation to help users of the final, unified model, understand the input parameters, file structure, and outputs. Each input parameter is described with units, typical maximum and minimum values, and the sensitivity of the output flow and sediment loads to it.

8. Calculated mass of pesticides present in the outflowing sediment. For every runoff event, a line is present in the output file GLEAMS_PEST.OUT that records the milligrams of each pesticide modeled that flowed off field with the sediment. This mass is calculated based on the concentration of pesticide in the top 1cm of the soil column.

9. Created Python script to convert CIMIS weather data to RZWQM meteorology input files. Script source and a pre-built windows executable are located in the 'cimis2rzwqm_script' directory.

10. Presented project results at DPR's offices in Sacramento. Presentation was live streamed to other interested parties. An online version of the presentation is located at http://ziram.lawr.ucdavis.edu/RZWQMGLEAMSpresentation/index.html and a snapshot of the presentation is available in the directory 'presentationRZWQMGLEAMSprintcopy'. To navigate the online presentation, use the left and right arrows to go back and forward in the slide stack respectively. Presentation was developed for Google Chrome, but should work on any HTML5 compliant browser.

11. Calibrated and validated models for:

- DPR alfalfa field trial
- Treynor IA multi-decade corn dataset
- Spanish olive orchard dataset

12. Drafted paper describing the integration of the two models. The paper contains the portions of this report describing each model, how they were integrated, and the results of calibrating and validating the model against real world datasets.

13. Drafted a poster for the 2014 ASA, CSSA, and SSSA Annual Meeting in Long Beach, CA describing in brief the project and results from the sensitivity analysis, calibration, and validation tasks.

14. Started preliminary work on 3D modeling tool: Using FEniCS for finite element modeling, I am implementing Fabian Bombardelli's[4] continuum mechanics based, complete two phase sediment model. Using this approach will create a pure physical model based on the conservation of mass and momentum. The continuum mechanics aspect allows for modeling the interaction of the highly viscous sediment laden baseflow and the lighter water dominated flow above it without resorting to extremely small cell sizes. This is important for an agricultural model because any flow offsite will be very shallow and thus the effects of the highly viscous baseflow will be more pronounced compared to a stream or river model. Eventually, the model meshes will be made using photogrammetry tools to convert photos of a field site into a 3D model. Plant geometry will be modeled using OpenAlea, then overlaid on the mesh to calculate sink and source values for water transport and soil chemistry.

Appendix B: Unpublished WEPP Work

WEPP

WEPP was developed by multiple U.S. Federal agencies during the mid to late 1980s to replace the USLE[2]. In contrast to the traditional formulation of the USLE, the WEPP sedimentation component can estimate spatial and temporal distributions of sediments loss and can predict sediment loss and deposition along a horizontal flow path of varying slope. In addition to the sediment routine, WEPP also models general hydrology, infiltration, and plant science. These routines are not used in this research; instead RZWQM is utilized for these tasks.

Rill erosion is estimated as a linear function of hydraulic shear stress while interrill erosion is estimated as a function of interrill slope and the square of rainfall intensity modulated by surface cover and plant canopy. Sediment transport in channels and rills is estimated using the Yalin equation[3].

$$\frac{T_c}{(SG)d\rho_w^{1/2}\tau_s^{1/2}} = 0.635\delta\left[1 - \frac{1}{\beta}\ln(1+\beta)\right]$$

$$\beta = 2.45(SG)^{-0.4}(Y_{cr})^{0.5}\delta$$

$$\delta = \frac{Y}{Y_{cr}} - 1(when\, Y < Y_{cr}, \delta = 0)$$

$$Y = \frac{\tau_s / \rho_w}{(SG-1)gd}$$

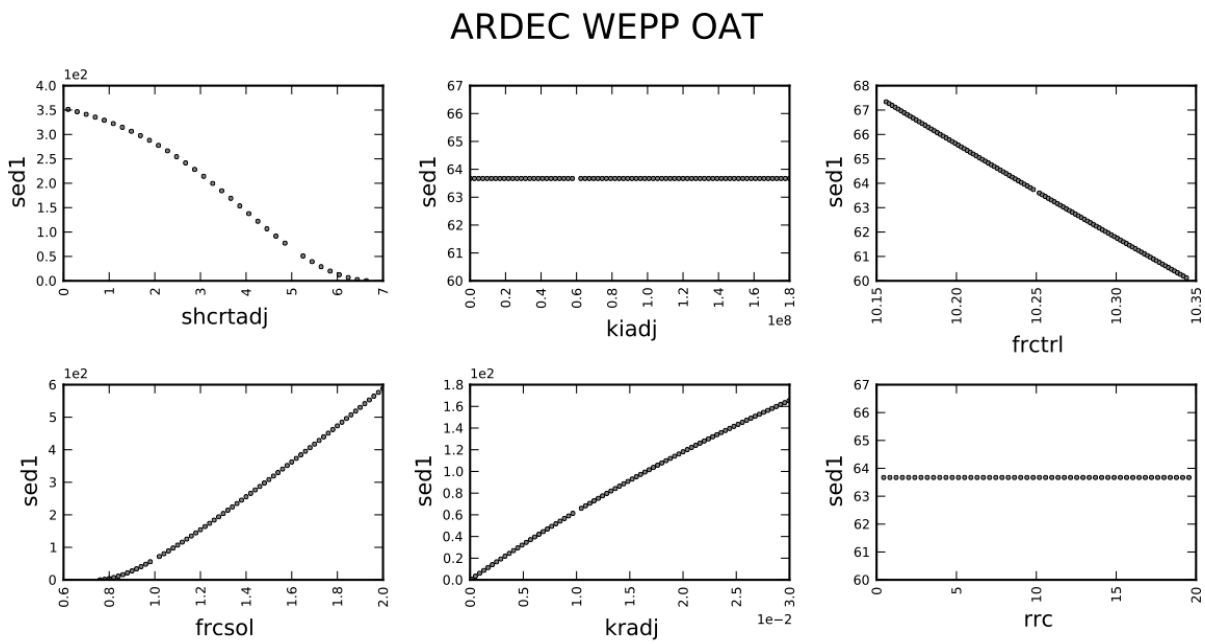
Where:

- T_c = sediment transport capacity
- SG = particle specific gravity
- ρ_w = mass density of water
- d = particle diameter
- Y = dimensionless shear stress
- Y_{cr} = dimensionless critical shear from Shields Diagram
- g = acceleration of gravity
- τ_s = shear stress acting to detach soil
- β and δ = dimensionless parameters as defined in the second and third equations respectively

Because the sediment routine in WEPP is more complex than the USLE based GLEAMS, more variables of possible concern exist. Some soil related parameters can be measured: diameter and specific gravity of each particle size, and how much of the total each particle size class represents. Other variables are synthetic factors similar to GLEAMS USLE variables discussed above and have no relation to field measured values: interrill and rill detachment rate parameters, critical shear stress, soil grain and rill friction factors, and the random roughness coefficient.

Initial Morris analysis of WEPP variables for both the ARDEC and DPR sites indicated that the adjusted interrill detachment rate parameter (kiadj) has no impact on sediment output for these specific models. The total rill friction parameter (frctrl) had a negative, linear relationship to sediment output. The adjusted critical shear stress (shcrtadj) had a slightly non-linear, negative relationship to sediment runoff while both the adjusted grain friction factor (frcsol) and the adjusted rill detachment rate parameter (kradj) had slightly non-linear, positive relationships to sediment runoff.

Sobol analysis indicated that the total rill friction parameter is by far the most sensitive parameter with regards to sediment flow. The only variable interaction of note is between the total rill friction parameter and the detachment rate parameter.



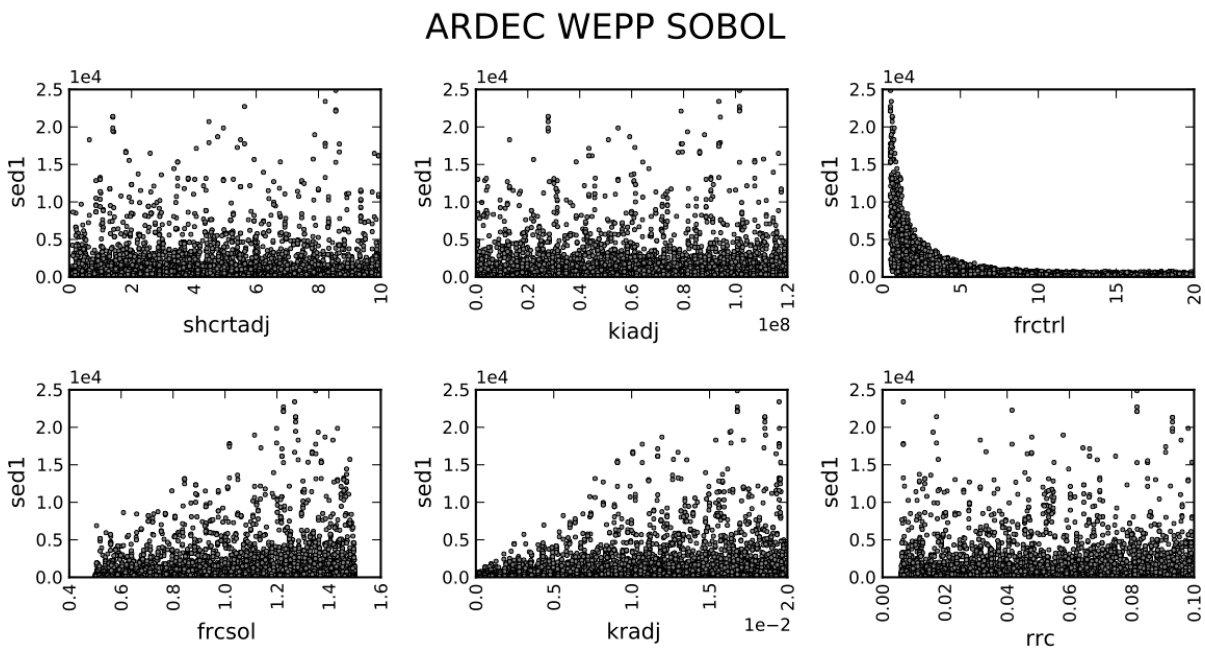


Table 1: WEPP parameters of interest

Name	Description	Units	Min Val	Max Val
spg	specific gravity of each particle size class			
frac	fraction of each particle class		0	1
dia	diameter of each particle class	mm		
kiadj	adjusted interill detachment rate parameter	kg/s/m^4	10000	12000000
kradj	adjusted rill detachment rate parameter	s/m	0.0001	0.02
shcrtadj	adjusted critical shear stress	kg/m/s^2	0.1	10
frcsol	soil grain friction factor	unitless	0.5	1.5
frctrl	total rill friction factor	unitless	0.5	20
rrc	random roughness coefficient	mm	0.006	0.1

Appendix C: Unpublished ARDEC (Agricultural Research Development & Education Center) Work

ARDEC Experimental Site

The research site is located in north central Colorado at the Colorado State University ARDEC complex, Ft. Collins, CO. Soil consisted of ARDEC sandy clay loam (55/16/29 Sand/Silt/Clay mix) with a 2% slope. During 2004, twelve simulation plots ($6m^2$, 2m wide by 3m long) were established and treated with differing amounts of constant and variable simulated rainfall over a 60min period. For each treatment, runoff and sediment yields were measured continuously at 5min intervals.

A RZWQM model was built using measured soil and environmental data, then calibrated by hand to match measured water inputs and output surface water flow. The amount of water supplied as precipitation was at the very limit of what was required for runoff given the most optimistic values for non-measured variables. Because of this, sensitivity analysis was completed using three consecutive days each with an hour of heavy rain, doubling in depth each day. This was done to ensure that there was runoff for most of the parameter space and to determine what effect precipitation amount had on the output

Appendix D: RZWQM-Sed Manual: to be inserted into the RZWQM manual (RZWQM2_User_Guide_APPENDIX_10_GLEAMS.docx)

APPENDIX 10: GLEAMS Data and Output Files – GLEAMS.DAT, GLEAMS_SED.OUT, Rzwqm-run.log

Erosion modeling is calculated using the sediment component of the Groundwater Loading Effects of Agricultural Management Systems (GLEAMS) model[1]. GLEAMS is an extension to the CREAMS model[2]. While there is a significant difference between GLEAMS and CREAMS with regards to pesticide fate and transport modeling; the erosion component remained largely unchanged. Both model sediment movement as a 1D horizontal set of linked reaches with the sediment loss of each reach governed by the Universal Soil Loss Equation (USLE)[3,4] slightly modified by CREAMS to model at the storm event time scale rather than an annual time scale. The USLE is a factor-based equation with each factor multiplied together to estimate soil loss. The value of each factor is determined through regression analysis of many field experiments performed by the USDA. The modified USLE is as follows:

$$D_{Li} = 0.210 \cdot EI \cdot (s + 0.014) \cdot K \cdot C \cdot P \cdot \left(\frac{\sigma_p}{V_u} \right)$$

$$D_{Fr} = 37983 \cdot m \cdot V_u \cdot \sigma \cdot p^{\frac{1}{3}} \cdot \left(\frac{x}{72.6} \right)^{m-1} \cdot s^2 \cdot K \cdot C \cdot P \cdot \left(\frac{\sigma_p}{V_u} \right)$$

Where:

- D_{Li} = interrill detachment rate (lb/ft^2/s)
- D_{Fr} = rill detachment rate (lb/ft^2/s)
- EI = Wischmeier's rainfall erosivity [100(ft-tons/acre)(in/hr)]
- x = distance down slope
- s = sine of slope angle
- m = slope length exponent
- **K = USLE soil erodibility factor [(tons/acre)(acre/100 ft-tons)(hr/in)]**

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[1] Leonard, Knisel, and Still, "Gleams - Groundwater Loading Effects of Agricultural Management-Systems."

[2] W. G. Knisel and K. R. Douglas-Mankin, "CREAMS/GLEAMS."

[3] Wischmeier, "Use and Misuse of Universal Soil Loss Equation."

[4] Renard et al., "RUSLE."

- **C = soil loss ratio of the USLE cover-management factor**
- **P = USLE contouring factor**
- V_u = runoff volume per unit area (ft)
- σ_p = peak runoff rate (ft/s)

Bolded parameters are those that can be changed by the user in the GLEAMS.DAT file. All other parameters are obtained from RZWQM.

Erosion is calculated daily for both interrill and rill areas with transport and deposition occurring during overland flow, channel flow, and in an optional impoundment. Parameters include slope and length of each channel and overland flow segment, USLE contouring and C parameters, and Manning's n values for any number of time periods during the modeled study.

When the GLEAMS.DAT input file is present in the scenario directory, sediment flow modeling is performed with output recorded in GLEAMS_SED.OUT and Rzwqm-run.log which describe the flow and sediment results in an abbreviated, easily parsable format and a detailed run log respectively. Pesticide mass flowing offsite is recorded in GLEAMS_PEST.OUT for each runoff event. If GLEAMS.DAT is not present, no sediment modeling is performed.

Overland sediment flow is computed along a 1D, horizontal line made up of at most ten different slope segments and up to four different segments with distinct USLE parameters. The USLE parameters can change on an annual basis over course of the model run. Optionally, channel erosion can also be modeled as a single channel accepting overland flow as input. The channel can have up to five different slope segments and four different USLE parameter segments.

When calibrating the model to measured outputs, RZWQM must first be calibrated to produce an accurate prediction of water runoff. Only once the surface water flow, the driving force of sediment runoff, is calibrated should individual GLEAMS parameters be calibrated to match observed sediment runoff.

For overland flow, the most sensitive parameters for sediment runoff are the field size and overall slope defined in rzwqm.dat, slope of each overland flow segment (SLOV), Manning's N (NFACT), and the USLE soil erodibility, cover management, and conservation practice factors (KFACT, CFACT, PFACT respectively). Analogous parameters exist for channel flow. Tables 1 and 2 display example values for CFACT and KFACT respectively. The conservation practice PFACT should be assigned a value of 1.0 if farming operations are uniform up and down the slope. If there is contouring only, PFACT is generally around 0.5. For contour strip farming, it is around 0.25. PFACT is the least reliable soil loss factor with no accepted table of example values.

The specific surface area of clay particles (SSCLY) has no effect on computed sediment runoff and can be set to any value between 20.0 for kaolinite to 800.0 for montmorillonite.

Figure 1: Ranges for significant GLEAMS parameters

Name	Description	Units	Min	Max

			Val	Val
SSCLY	Specific surface area for clay particles Suggested values: 20.0 for kaolinite, 800.0 for montmorillonite	m^2/g	20	800
KSOIL	Soil erodibility factor for the slop segment just above start of model	ton/ac or t.ha.h/ha.MJ.mm	0.001	0.08
CFACT	Soil loss ratio for overland flow profile segment	unitless	0	0.4
PFACT	Contouring factor for overland flow profile segment	unitless	0.01	1
NFACT	Mannings 'n' for overland flow profile segment.	unitless	0.01	0.14

Table 2: Typical C-Factors from “Soil Erosion by Water.”

Table 3: Typical K-Factors for a number of cropland, rangeland and forest soils from “Soil Erosion by Water”

```
=UF-Erosion-ADDENDUM
=====================================================================
==                                                                 ==
==                GLEAMS E R O S I O N   M O D E L                ==
==                 MODEL VARIABLES AND PARAMETERS                  ==
==                                                                 ==
=====================================================================
=     Erosion control parameters
=
=     See GLEAMS documentation for more detailed descriptions.
=
= ITEM NO.   DESCRIPTION
= --------   -----------
= TITLE      Three 80-character lines of alphanumeric information
=            that identifies the particular computer run.
= WLW        Watershed length::width ratio
=            WLW = LFP^2 / (DAREA * 10000) [DAREA=ha, LFP=longest flow path [m]]
= FLGSEQ     Flag indicates the execution sequence of erosion-sediment
=            sub-models as follows:
=                  1  overland
=                  2  overland-impoundment
=                  3  overland-channel
=                  4  overland-channel-channel
=                  5  overland-channel-impoundment
=                  6  overland-channel-channel-impoundment
= SSCLY      Specific surface area for clay particles (m^2/g)
=            Suggested values: 20.0 for kaolinite, 800.0 for montmorillonite
= NPTSO      Number of points for overland flow profile slope (Max = 10)
= DAOVR      Drainage area represented by the overland flow profile [ha]
= XOV(nptso) Distance from upper end of overland flow profile to the point
=                  where slope is given. [m]
= SLOV(nptso)Slope of the overland flow profile at the XOV. m/m
= NXK              Number (1 to 4) of slope segments differentiated by changes in
=                  soil erodibility factor
= XSOIL(nxk) Relative horizontal distance from top to bottom of the slope.
=                  Last value must be 1.0.
= KSOIL(nxk) Soil erodibility factor for the slop segment just above XSOIL
=                  Units = t.ha.h/ha.MJ.mm
= NSC              Number of channel segments differentiated by changes in slope
=                  (max = 5)
= CTLO       Channel outlet control condition that affects flow depth:
=                  1  critical depth controls depth at the end
=                  2  uniform flow controls depth at the end
=                  3  same as 2, except Manning's 'n' for the outlet
=                     is the same as that for the lower segment of
=                     the field channel; the field channel continues
=                     beyond the edge of the field.
=                  4  a rating curve controls depth at the end
=                     Critical discharge, Q, is computed as follows
=                     Q = RA * Y^RN
=                         Q = critical discharge; ft/s or m/s
=                         RA = coefficient
=                         Y = flow depth; ft or m
=                         RN = exponent
= RA         Coefficient in rating equation. Leave blank if CTLO < 4
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= RN         Exponent in rating equation. Leave blank if CTLO < 4
= DACHL      Total drainage area at the lower end of the channel. [ha]
= DACHU      Drainage area at the upper end of the channel. [ha]
= Z          Side slope of the field channel cross-section expressed as
=            horizontal to vertical distance: [m/m].
=            Enter the value for Z that most closely approximates the
=            channel shape
= XLSP(nsc)  Distance from upper end of the channel to the bottom of segment
=            Units = [m]
= SSLP(nsc)  Slope of segment directly above. [m/m]
= CTLZ Side slope of a cross-section of the outlet control channel,
=            ratio of horizontal to vertical
= CTLN Mannings 'n' for the outlet control channel
= CTSL Slope of the outlet control channel [m/m]
= NYEARS     Number of years in this rotation
= CDATE(10)  The Julian days on which sets of parameters take effect.
= NXF        Number (1 to 4) of overland flow profile segments
=            differentiated by changes in the overland flow updateable
=            (annual) parameters
= XFACT(nxf) Relative horizontal distance from the top of the overland flow
=                  profile to the bottom of segment (ratio of distance to bottom of
=                  segment to total profile length)
= CFACT(nxf,nyears) Soil loss ratio for overland flow profile segment
= PFACT(nxf,nyears) Contouring factor for overland flow profile segment
= NFACT(nxf,nyears) Mannings 'n' for overland flow profile segment.
=                        must never be less than 0.010
= NXC        Number (1 to 4) of channel profile segments differentiated by
=            changes in the channel parameters
= XCHAN(nxc) Relative horizontal distance from top of channel to bottom of
=                  segment
= NCHAN(nxc,nyears) Mannings 'n' for channel segment
= DCHAN(nxc,nyears) Depth to nonerodible layer in the middle of the channel
= WCHAN(nxc,nyears) Top width of channel
=========================================================================
*** Overland only flow from an alfalfa field with calibrated CFACT, PFACT, & NFACT
12.5                                                    [WLW]
1                                                          [FLGSEQ]
20.0                                                    [SSCLY]
1  0.27                                                 [NPTSO,DAOVR]
198.12  0.0014                                          [XOV(nptso),SLOV(nptso)]
1  1.0  0.86241                                         [NXK,XSOIL(nxk),KSOIL(nxk)]
1                                                       [NYEARS]
001 -1  -1  -1  -1  -1  -1  -1  -1  -1                  [CDATE(10)]
1  1.0                                                  [NXF,XFACT(nxf)]
0.016804                                                   [CFACT(nxf)/1/1]
1.0                                                     [PFACT(nxf)/1/1]
0.003385                                                [NFACT(nxf)/1/1]
```

Appendix E: Model Integration & Sensitivity Analysis Paper (integration_sa_paper.docx)

Integrating GLEAMS sedimentation into RZWQM for pesticide sorbed sediment runoff modeling

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Abstract

This study integrated the sediment and surface flow components of Groundwater Loading Effects of Agricultural Management Systems (GLEAMS) model into the Root Water Quality Model (RZWQM) to create a derivative model named RZWQM-Sed. After integration, a sensitivity analysis was performed to determine which variables had the greatest influence on water and sediment flow off field. The integrated model was calibrated and validated against multiple real world datasets spanning a range of space and from catchment sized multi-decade trials to single fields studied for a couple of years. The integrated model did a good job predicting the mass of sorbed chemicals in the tailwater (Nash-Sutcliffe coefficient > 0.3), was no better than using a past average in predicting average sediment loss from small fields for a single runoff event (NS around zero), and was unimpressive in predicting sediment loss from a catchment on a year to year basis (NS less than zero).

Introduction

Sediment runoff is a significant environmental problem that negatively impacts native ecosystems, the parent soil column, as well as manmade hydrologic infrastructure. In addition to the problems resulting from the inert sedimentary soil particles themselves, agricultural sediment runoff is even more problematic due to the additional toxic chemicals sorbed to the mobile sediment particles. In order to evaluate best management practices which seek to minimize sediment and sorbed chemical runoff from agricultural land uses, it is imperative to have a model that tracks hydrologic processes, plant growth kinetics, bulk soil movement, and solute chemistry in a unified setting. Currently available models are weak in one or more of the above requirements. It is therefore necessary to seek solutions through integrating features from existing models or developing new models that can accurately model chemically sorbed sediment runoff.

Sediment models, like any other computational modeling of natural systems, can be classified as empirical, conceptual or physical. Empirical models algebraically combine a small handful of parameters whose values are determined through regression from field data or are easy to measure physical quantities. The benefit of empirical models is that the amount of input data is quite small and calculations are very quick. The Universal Soil Loss Equation (USLE)[1] is an empirical model that forms the basis of many current sediment models. In this equation, soil loss is computed on an annual basis calculated by the multiplication of six factors (rainfall erosivity factor, soil erobibility factor, flow length, steepness, crop/cover management factor, and conservation factor) representing five physical items: rainfall, soil, slope and length of the flowline, and land cover. These factors are derived from a regression analysis of field research site data. Subsequent models, like the Revised Universal Soil Loss Equation (RUSLE)[2], extended the USLE to handle some seasonal variation and sub-annual time steps. PERFECT[3], CREAMS[4], and CREAMS' successor GLEAMS[5] also utilize a version of the USLE modified for sub-daily time steps.

Conceptual models are middle ground between empirical and physical models. The system being modeled is broken down into multiple interacting pools, with pools representing everything from water storage to nitrogen to microbial communities. There are governing equations that track the movement and transformation of substances being studied within each pool and between pools. While conceptually there is some scientific merit behind the equations linking the various storage pools, they still represent averaging abstractions that have only a tenuous link to the physics of what is actually going on in the system studied. Examples of conceptual sediment models include: AGNPS[6], EMSS[7], LASCAM[8], and SWRRB[9]. These models tend to be designed to work for large regions, catchments and above, over lengthy time scales. The more time and space is averaged through larger timesteps and coarser computation grids, the easier it is for most empirical and conceptual models to match measured values of real world systems.

Physical models start with first principles (conservation of mass, momentum, heat, etc) which are translated into partial differential equations and subsequently solved via a numerical method. These models tend to require a large amount of input data, some of which might be impossible to measure in the field, and are extremely computationally intensive. Provided that the necessary input data can be obtained, physical models have the possibility of being the most accurate over the whole domain, from stream bed to watershed spatial scales, and can follow an arbitrary time and space discretization. Examples of sediment models that claim to be at least partially physically based include ANSWERS[10], GUEST[11], HSPF[12], LISEM[13], and WEPP[14].

Most of the claimed physical models listed above are not purely physical; they have a portion of their calculations depend on empirically based values. For instance, WEPP uses Foster's equations for sediment transport calculations which sets the sediment rate per unit width of rill channel to the summation of rill and interrill detachment/deposition rates. These rates must be derived from empirical equations based on soil type, topography, land cover and other factors. GUEST uses the Rose equation which includes factors for volumetric flux of water, runoff rate, rainfall rate, rill density, available depositional area, rill to

interrill transfer, and the wetted perimeter. But it depends of user supplied factors like the rainfall erodibilty parameter and the fraction of streamflow power effective in re-entraining sediments. ANSWERS uses an empirical equation to calculate soil particle detachment and the bedload transport equation to predict the transport of non-cohesive grains. LISEM utilizes Grovers'[15] rill transport equation which depends on two experimental coefficients (c & d) that vary depending on the median texture (d50) of the soil material.

An ideal agricultural sediment model would be able to function across time and space scales, require a minimal number of input variables, and calculate quickly. Speed of execution is somewhat flexible provided that the code can make use of multiple processors as cost per FLOPS has been on a constant linear decline. Tracking the fate and transport of decaying sorbed chemicals requires a field level spatial scale and a time scale on the order of hours or less. Calculating the bulk soil loss from rangeland necessitates a watershed spatial scale and a monthly or even yearly time scale. Often models will work best at a specific time and space scale while producing unacceptable results for other scales.

The sediment models listed above lack the robust plant growth kinetics, soil chemistry, and pesticide fate and transport modules that are present in the Root Zone Water Quality Model (RZWQM)[16].

RZWQM is a mechanistic model designed to simulate plant growth and movement of water, nutrients and pesticides in an agricultural system. The model has been widely used around the world to simulate water and agrochemical movement as impacted by different management practices. It has been recently enhanced by improving the pesticide sub-model, which includes detailed algorithms for simulating pesticide transport and fate in four (4) compartments: crop foliage, crop residues, soil surface and soil sub-surface or root zone.

While RZWQM is a well studied, heavily used, agricultural processes model with a focus on plant growth kinetics and solute transport, it unfortunately lacks a sediment runoff component. To alleviate this hole in sediment modeling, RZWQM and GLEAMS, two models with complementary capabilities, were merged

to form a unified model. The objective of this study was to integrate the sediment routine from GLEAMS into RZWQM in order to fill the gap in functionality identified above, determine what variables of the unified model are the most important to water and sediment runoff, then test the integrated model against multiple real world datasets in order to assess the model's accuracy across time and space scales.

Materials & Methods

RZWQM

In the mid 1980s, scientists at the USDA Agricultural Research Service (ARS) determined that there was a need for a model that could track water quality through the unsaturated vadose zone in agricultural environments. After reviewing such contemporary models as NTRM, CREAMS, and PRZM, the team designed a model that included features needed for tracking farm processes including chemical transport via macropores, tile drainage, soil chemistry and nutrient transformations, advanced pesticide dynamics, plant growth modeling and management options for water and chemical applications. The first model was completed in 1992. Subsequently, the model has been extensively tested and refined with additional plant growth and chemical tracking modules added over the years along with the Windows based GUI. The version of RZWQM used for development in this study is Version 2.5, supplied by ARS. A detailed description can be found in Ahuja et al.[16]

RZWQM is a one dimensional (vertical) model with the ability to discretize the soil column into up to twelve different user defined, uniform layers. Internally, the model uses 1cm thick layers for numerical modeling. The major processes of plant growth, soil chemistry, nutrients, pesticides, site management, and evapotransporation operate on a daily time scale while heat transport, water balance, solute transport, snowpack dynamics, and chemical uptake operate on a sub-hourly time scale.

Infiltration is modeled using a Green-Ampt equation[17] modified to include surface crust simulation based off the work of Bouwer[18], Morel-Seytoux and Khanji[19], and Brakensiek and Onstad[20]:

$$V = \frac{K_s}{2} \cdot \frac{\tau_c + H_0 + Z_{wf}}{Z_{wf}}$$

Where:

V = infiltration rate (cm/hr)

K_s = effective average saturated hydraulic conductivity (cm/hr)

τ_c = capillary drive at the wetting front (cm)

H_0 = depth of surface ponding

Z_{wf} = depth of the wetting front.

A viscous resistance correction factor of 2 is used to correct the effect of entrapped air on K_s due to surface crusts.

Movement of water through the soil column post infiltration is calculated using a slightly modified Brooks-Corey[21] equation to quantify the relationship between soil water content vs. the matric suction.

$$\theta(\tau) = \theta_s - A_1\tau; \tau \leq \tau_b$$

$$\theta(\tau) = \theta_r - B\tau^{-\lambda}; \tau > \tau_b$$

Where:

Θ = volumetric soil water content (cm^3/cm^3)

τ = matric suction head (cm, $\tau = |h|$, where h is the soil water pressure head)

Θ_s = saturated soil water content (cm^3/cm^3)

Θ_r = residual water content (cm^3/cm^3)

τ_b = air-entry or bubbling suction head (cm)

A_1, B, and λ are constants, though B is not an independent parameter, it is determined from other parameters by the condition of continuity at $\tau = \tau_b$.

The hydraulic conductivity vs matric suction relationship is:

$$K(\tau) = K_s \tau^{-N_1} ; \tau \leq \tau_{bK}$$

$$K(\tau) = K_2 \tau^{-N_2} ; \tau > \tau_{bK}$$

Where:

- K = hydraulic conductivity (cm/hr)
- K_s = field-saturated hydraulic conductivity (cm/hr)
- τ_{bk} = air-entry or bubbling suction head for this function (cm), which may equal τ_b introduced above.

Once surface water application exceeds the maximum soil infiltration rate, runoff is produced as a runoff depth. Total runoff is calculated by multiplying the runoff depth by the field area.

Surface water runoff volume is the most significant variable for sediment loss; therefore the RZWQM parameters of most concern are those that effect infiltration and thus directly affect calculated runoff. Most of the variables listed in Table 6 can be measured in the field or via laboratory analysis of soil samples, but some like ct, eps, and lamda are abstract variables with no true relationship to a value that can be measured in a field or a laboratory.

GLEAMS

The GLEAMS model was chosen for the sediment component because of its well documented history of successful use, it requires minimal input variables above and beyond those already required by RZWQM, and it requires minimal computation time per runoff event.

GLEAMS[5] is an extension of the CREAMS model[22] developed during the 1980s at the U.S. Department of Agriculture, Agricultural Research Service. While there is a significant difference between GLEAMS and CREAMS with regards to pesticide fate and transport modeling, the erosion component remained relatively unchanged. Both model sediment movement as a 1D horizontal set of linked reaches with the sediment loss of each reach governed by the Universal Soil Loss Equation (USLE)[1] as modified by CREAMS for storm-by-storm modeling.

$$D_{Li} = 0.210 \cdot EI \cdot (s + 0.014) \cdot K \cdot C \cdot P \cdot \left(\frac{\sigma_p}{V_u} \right)$$

$$D_{Fr} = 37983 \cdot m \cdot V_u \cdot \sigma \cdot p^{\frac{1}{3}} \cdot \left(\frac{x}{72.6} \right)^{m-1} \cdot s^2 \cdot K \cdot C \cdot P \cdot \left(\frac{\sigma_p}{V_u} \right)$$

Where:

- D_{Li} = interrill detachment rate (lb/ft^2/s)
- D_{Fr} = rill detachment rate (lb/ft^2/s)
- EI = Wischmeier's rainfall erosivity [100(ft-tons/acre)(in/hr)]
- x = distance down slope
- s = sine of slope angle

- m = slope length exponent
- **K = USLE soil erodibility factor [(tons/acre)(acre/100 ft-tons)(hr/in)]**
- **C = soil loss ratio of the USLE cover-management factor**
- **P = USLE contouring factor**
- V_u = runoff volume per unit area (ft)
- σ_p = peak runoff rate (ft/s)

The USLE is a factor-based equation with each factor multiplied together to come up with an estimation of soil loss. The value of each factor is determined through regression analysis of many field experiments performed by the USDA. Initially the USLE only operated on an annual time step, but modifications over the years have allowed the model to run over a per storm time step, which was the time step utilized by the joint model.

Erosion is calculated daily for both interrill and rill areas with transport and deposition occurring during overland flow, channel flow, and in an optional impoundment. Parameters include slope and length of each channel and overland flow segment, USLE contouring and C parameters, and Manning's n values for any number of time periods during the modeled study. The only parameters in the modified USLE that can be changed by the user are bolded above. These USLE factors cannot be measured in the field; at best they can be looked up from published tables based on sites with similar soil, crops, and management.

Site Descriptions

Three study sites were chosen: a two year experimental alfalfa study in Davis, CA that focused on offsite sediment and solute transport, a three year study of an Olive orchard in Cordoba Spain that only focused

on sediment flow off field, and a three decade study of a corn planted watershed in Treynor, IA that was also only interested in offsite sediment and water flow (Figure 14).

Site 1: Alfalfa Field Experiment in Davis, California

Two alfalfa fields (0.27ha each, 15.8m wide by 198.12m long) in Davis, California were use for the experiments. Soils in the study consisted of Yolo silty loam (35/40/25 Sand/Silt/Clay mix) with a 0.14% slope. There were seven flood irrigation events during 2012 and four during 2013 with input and output flow measurements taken every 2min and sediment measurements taken approximately every 30min. Most irrigation events applied around 3cm of water to the field, with one event applying 11cm. Rain was negligible during the months when measurements were made. Along with sediment, sorbed pesticides previously applied to the field were measured in the runoff: one trial utilized Chlorpyfios, the other Diuron.

Site 2: Watershed Scale Corn Experiment in Treynor, IA

To model watershed scale effects on a time scale in the decade range, this study used annual data from the Deep Loess Research Station located near Treynor, Iowa. The silt-loam soils are classified as Typic Haplorthents and Cumulic Hapludolls with fine silty, mixed mesics and have moderate to moderately rapid permeability. Average slope is around 8 to 9 percent with a maximum slope of 18 percent. The watershed area is 30.4ha. Corn was grown throughout the study time period which spanned the years between 1964 and 1996. No irrigation was performed. Precipitation was left unmodified from the measured values. While the model was run over sub-daily time steps, calibration and validation was done using yearly summations in order to match the format of available field data.

Site 3: Olive Orchard Experiment in Cordoba, Spain

Data from this model was obtained from the paper by Taguas et al[23]. The study site is an olive planted microcatchment 6.1ha in size located in the south-west of the Province of Cordoba, Spain (37.4°N, 4.8°W) with a mean elevation of 239m and mean slope of 15%. The soil is Cambisol, a loamy sand soil

with an organic matter content of 1.6% and bulk density of 1.61g/cm^3. Olive trees were planted in 1999 with 7m of space between each tree. Rainfall, runoff, and sediment loads were recorded from May of 2005 to February of 2008 at daily timesteps. No irrigation was applied; all water input was from rainfall.

Integration of the RZWQM and GLEAMS

The GLEAMS sediment module requires the following data for each runoff event: bulk density of soil particles, the field's acreage and length-to-width ratio, average temperature, total rainfall, excess rain, intensity of excess rain, and the proportion of clay, silt, sand, and organic matter in the soil. During initialization, parameters that are shared between RZWQM and the sediment modules, such as soil composition and field geometry, are set by RZWQM to be later used by the sediment component. Parameters specific to the sediment component are read from a dedicated input file. The GLEAMS sediment routine is called from RZWQM whenever a precipitation or irrigation event occurs that results in surface runoff. GLEAMS then calculates the bulk soil loss and outputs results to five text files. In addition to a detailed output log shared with the parent code base, the sediment component writes a readily parsable table of output values with one row per day that runoff occurred to four different files: one for water and sediment flow, and one each for the three possible pesticides to track sorbed solute flow off field. Each row of water and sediment flow output contains: the calculated surface water runoff, total sediment runoff (expressed in both tons per hectare and volumetric concentration), and sediment loss for each class of particle size. The calculated sediment output from GLEAMS is then used within RZWQM to estimate the mass of modeled pesticides dissolved in the tailwater as well as the mass of pesticides in different soil bound pools distinguished by how mobile the solute is. Input and output through plain text files is the standard way to interact with both base models and has been maintained for the unified model.

RZWQM and GLEAMS are both written in Fortran. They were compiled for this study on Windows 7 using Intel Fortran and Microsoft Visual Studio. Currently, the unified model is command line only and the parameters of sediment component can only be set using a plain text file. The RZWQM portion of the model can still be set up using the existing GUI, then the sediment input text file can be added to the

project directory. If the sediment input file is present when the model is run, then the GLEAMS sedimentation routine is executed, otherwise only the RZQWM routines are executed. The next public release of RZWQM should incorporate the sediment component and include a GUI input menu for the GLEAMS parameters.

Sensitivity Analysis

After integrating RZWQM and GLEAMS, a sensitivity analysis was performed on the integrated model to determine which variables have the greatest influence on modeled surface water flow and sedimentation. In order to understand a model well enough for it to be properly used, it is necessary to conduct a sensitivity analysis for the input parameters. A sensitivity analysis identifies factors or groups of factors most responsible for variation in model output and thus most responsible for uncertainty in the model's prediction. Particular attention was paid to the variables that are coefficients in the governing equation which do not correspond to a physical measurement. A two stage sensitivity analysis was performed separately for both the variables effecting surface water runoff and variables effecting sediment runoff. The first stage utilized a Morris style one-at-a-time analysis to identify variables with no influence. Following that, a Sobol sensitivity analysis was performed on the remaining variables to quantify their influence and determine if there was any interaction between pairs of variables that didn't present itself in the single variable analysis. Knowledge gained from this sensitivity analysis was utilized during the calibration and validation of the integrated model so that only the variables of import were calibrated while those of little import were left fixed. For runoff, residual and saturated water content along with Brooks-Corey bubbling pressure had the greatest influence. Universal Soil Loss Equation factors and Manning's N showed the greatest influence for modeled soil loss.

Previous sensitivity analyses for either RZWQM or GLEAMS did not target the parameters of interest to this project. A sensitivity analysis of GLEAMS was done by Cryer et al[24] using a factorial design technique and focused on solute pesticide transport, ignoring sediment transport. Persicani[25] ran a sensitivity analysis on GLEAMS, MOUSE, TETRANS, and HYDRUS, but only used the Morris method.

Wedwick et al[26] performed both a Morris and Monte-Carlo sensitivity analysis on a irrigation extension of GLEAMS called GLEAMS-IR, but didn't investigate sedimentation. Ahmed et al[27] performed a Morris sensitivity analysis, then calibration and validation of RZWQM on two sites in Ontario, Canada.

Two generalized models were built for sensitivity analysis, both based off of the DPR alfalfa experiment. One site had the simulated alfalfa while the other was bare soil, otherwise they were identical. Sensitivity analysis results were similar enough that only the results from the planted model are presented with any differences between the two noted.

Surface water runoff is the main driver sediment loss; therefore the RZWQM parameters of most concern are those that effect infiltration and thus directly affect calculated runoff. All variables relating to infiltration are listed in Table 6. Most of the variables listed in that table can be measured in the field or via laboratory analysis of soil samples, but some like ct, eps, and lamda are abstract variables with no true relationship to something that can be measured in the field or laboratory.

The variables of interest for the GLEAMS sedimentation routine are listed in Table 5. Aside from the slope profile which can be measured in the field, the most interesting sedimentation variables are the USLE C, P, and N factors and possibly the specific surface area of clay particles. The latter was included primarily because it is hard to accurately measure; therefore it is imperative to know if its value effects sediment flow.

Sensitivity Analysis Methods

One-At-A-Time Morris

The oldest and most widely used in published literature, sensitivity analysis method is the Morris One-At-A-Time method (OAT)[28]. This method starts with a default value for each variable, and then modifies a single variable per model run with all other variables set to their default value. OAT is quick to run and easy to implement. This method never makes type 1 errors: a non-zero effect implies influence of that variable on the output.

Unfortunately there are many problems with relying on OAT alone. Underlying OAT are several fundamental assumptions that might not hold for complex models: OAT assumes model linearity and total variable independence. Furthermore, OAT sensitivity analysis cannot sample the whole problem space; if all variables are independent and the domain is normalized to the unit hyper-cube, OAT will only sample within the unit hyper-sphere. With two variables, OAT can sample 78% of the domain. With twelve variables, OAT can only sample 0.0326% of the domain.

Sobol

Sobol sensitivity analysis (also known as the variance method) samples the whole domain and quantifies the total influence of each variable singularly as well as the effect of multi- variable interactions.[29] For a simple example with only three uncertain parameters the total variance is:

$$V(Y) = V_1 + V_2 + V_3 + V_{12} + V_{23} + V_{13} + V_{123}$$

The first order sensitivity index is:

$$S_i = \frac{V_{X_i}\left(E_{X_{\hat{i}}}(Y \mid X_i)\right)}{V(Y)}$$

The total order sensitivity index, which includes parameter interaction effects, is:

$$S_{Ti} = \frac{E_{X_{\hat{i}}}\left(V_{X_i}(Y \mid X_{\hat{i}})\right)}{V(Y)}$$

Where:

- Xi = the i-th factor
- Xî denotes the matrix of all factors but Xi
- Inner expectation operator: the mean of Y (scalar output of interest) is taken over all possible values of Xî while keeping Xi fixed.
- Outer variance is taken over all possible values of Xi

- The variance V(Y) in the denominator is the total unconditioned variance.
- VXi(EXî(Y|Xî)) is the expected reduction in variance that would be obtained if Xi could be fixed.
- EXî (Vxi(Y|Xî)) is the expected variance that would be left if all factors but Xi could be fixed.
- Si gives the effect of factor Xi by itself
- STi gives the total effect of a factor inclusive of all its interactions with other factors.
- For additive models: Si = STi

Domain sampling can be done either using a simple Monte-Carlo approach, Latin hyper-cube sampling, or a Sobol sequence[30]. The latter approach was used in order to sample the domain as completely as possible while still maintaining pseudo-randomness and requiring less model runs compared to the other methods.

RZWQM Sensitivity Analysis Results

Initial OAT analysis of the variables associated with infiltration showed no response for either study site for the following: 1/3 and 1/10bar field capacity, wilting point, the second intercept on the K(h) curve, and lateral hydraulic conductivity (See Figure 2). The exponent for the K(h) curve had a linear response, while the remaining variables displayed a non-linear response.

Table 8 shows the results, sorted by total order effect, of the Sobol analysis of RZWQM variables that showed an influence during OAT analysis. Residual water content, saturated water content, and bubbling pressure from the Brooks-Corey equation showed the highest influence for both models followed by the saturated hydraulic conductivity and the non-Brooks-Corey bubbling pressure. None of the total order results show a dominant influence (total order > 0.8).

Analysis of second order effects reveled minor variable interaction effects between residual and saturated water content and between residual water content and Brooks-Corey bubbling pressure for both sites. These effects were more pronounced when the modeled site was bare soil rather than a planted field.

GLEAMS Sensitivity Analysis Results

There was no evidence that the specific surface area of clay particles (sscly) had any effect on sediment output. The USLE parameters cfact, pfact, and ksoil had an expected positive linear relationship to soil loss up until a ceiling where maximum output was reached and increasing the variables' value no longer had an effect. This ceiling was model dependent, and was only obvious on the unplanted site. Manning's N (nfact) showed an opposite response: constant sediment flow from zero nfact to a model dependent threshold, then a quick, exponential decay to zero sediment flow.

Scatter plots from Sobol runs showed similar results. The plots of USLE factors filled in the area under the line formed in the OAT analysis. Manning's N behaved similarly for the unplanted ARDEC site, filling in the space below the decay curve, but for the study planted with alfalfa, there were several points above the curve boundary where there was sediment flow.

Analysis of the Sobol statistics (Table 7 and Figure 3) also displayed a stark difference of the influence of Manning's N between the planted and unplanted models: it dominated the unplanted model and was least influential in the planted model. The USLE factors have a predictably equal and significant influence on the output.

Calibration

The Design Analysis Kit for Optimization and Terascale Applications (DAKOTA)[31] package, developed at Sandia National Labs, was used for automated calibration of each model against measured data in a two stage process. First, surface water flow was calibrated by modifying the RZWQM variables shown, via sensitivity analysis, to have an influence on runoff. Then the sediment model was calibrated using the RZWQM parameter values found in step one and varying the influential sedimentation parameters

identified during sensitivity analysis. Optimization was completed using a global, gradient free, genetic algorithm[32] included with the DAKOTA package using parameters in Table 4.

Validation

The DPR alfalfa trial was irrigated via flood irrigation. RZWQM is a one dimensional model; therefore, the only flood irrigation method that is supported is rice-paddy style stagnant ponding. In order to model the flowing flooding of the alfalfa fields in this study, the model's irrigation input was hand calibrated so that calculated output flows matched measured values. This isolated the sediment sub-model from any errors that RZWQM's runoff calculations might introduce, but made it impossible to assess RZWQM's runoff calculations. The field trial included two neighboring blocks of planted alfalfa that were individually monitored for water, sediment, and chemical runoff over two years. One block was used for calibration over the whole study period while the other block was used for validation.

Unlike the alfalfa trial, the other two sites used for calibration and validation only had data available for a single field; therefore they were calibrated against the first half of available data and validated against the remaining data. The Treynor site model was calibrated to the years 1964-1978 and was then validated against the remaining years. The Spanish olive model was calibrated to the first two years, and then validated against the last two years of data. Both the Treynor corn trial and the Spanish olive trial were rain irrigated only, therefore RZWQM parameters were calibrated to measured outflow for a given time period using measured precipitation, then these parameters were validated against the other time period providing an indication on the performance of the RZWQM runoff calculations.

Results

Site 1: Alfalfa Field Experiment in Davis, California

Charts comparing measured versus modeled water and sediment flow at the Davis DPR site are presented in Figure 6 and Figure 7 respectively with a tabular version of said data in Table 9. Sediment flow error statistics are presented in Table 14 and Table 15. Solute flow graphs are presented in Figure 8 and Figure 9, while error statistics are presented in Table 16 and Table 17. As mentioned before, water runoff was hand calibrated to measured data by modifying the amount of water input while keeping the RZWQM parameters set at constant, conservative values. This isolates the sediment routine so that the accuracy of bulk sediment runoff and mass of sorbed chemicals can be assessed in an annual field environment. Even with the runoff hand optimized, sediment flow results were not that impressive: over 100% average percent error and a negative Nash Sutcliffe coefficient. There is minimal difference in sediment flow from event to event with all flows clustering tight around the mean. While the sensitivity analysis of the sediment model did show an expected high sensitivity to water input, the differences in water input given the other parameters resulted in minimal change to sediment output.

The lack of significant variation in modeled sediment output given the range of water flows might not be as problematic as it seems: the natural variability might depend on a process that is not, or cannot, be modeled. The irrigation on 2012241 had around four times as much water as any other irrigation event, yet the measured sediment was one of the lowest. The next irrigation event (181 days later) had the highest sediment runoff despite having only an average water input. Other factors, like the condition of the canal where measurements took place or wind deposited silt from offsite, could be behind these curious differences. These unknown factors might never be known and if they were, might be impossible to model under the RZWQM framework.

On a more positive note, sediment sorbed pesticide results were visually better than the DPR alfalfa results with predicted values tracking measured values rather well. The 2013057 diuron trial was the only

one that showed an extreme spread between measured and modeled. Given how much larger the measured mass was on this trial versus all the other measurements, it might indicate some sort of measurement error. Or, given that the concentrations are less than one part per billion, it could be simple chance that more slightly more particles of Diuron were entrained in that sample compared to another. When that trial is removed, the average percent error drops to 59% and the Nash Sutcliffe coefficient becomes a very strong 0.74. The chlorpyrfios trials have no obvious outlier and a respectable Nash Sutcliffe coefficient of 0.39. The average absolute error is pretty high at 720%, but that drops to 152% with the removal of trial 2012241 which has a 3,560% error. This is the last measurement made for a given chlorpyrfios application and the measured mass was close to zero.

Site 2: Watershed Scale Corn Experiment in Treynor, IA

The results from the Treynor study site are described in Figure 4, Figure 5, Table 10,

Year	Measured (cm)	Modeled (cm)
1964	15.82	18.09
1965	34.77	18.84
1966	7.21	17.50
1967	34.39	14.10
1968	6.58	11.30
1969	13.41	16.75
1970	10.29	15.45
1971	17.09	16.17
1972	9.70	20.42
1973	24.56	11.99
1974	15.57	14.09
1975	12.98	20.10
1976	9.12	13.48
1977	22.07	17.87
1978	18.06	13.04
1979	19.99	14.16
1980	18.08	20.66
1981	7.09	10.52
1982	20.68	14.38
1983	20.55	16.02

1984	34.90	12.82
1985	13.08	15.71
1986	21.41	11.79
1987	24.84	13.24
1988	8.94	16.88
1989	9.53	16.87
1990	5.69	18.28
1991	17.09	8.01
Avg	16.91	
NS	-0.27	

Table 11, Table 12, and. Predictions of water flow were unimpressive for either the calibrated or validated dataset with an average percent error of around 100% and a Nash Sutcliffe coefficient of -0.5 to -0.3 depending on if possible outliers are removed or not. A Nash Sutcliffe coefficient less than one indicates that the model is a worse predictor than just using an average of past data. This isn't that surprising since validation and calibration was done using annual measured data compared to a summation of RZWQM calculated events for that year. Care should be taken when using RZWQM for very long time periods, especially there are no individual runoff events to calibrate against as even slight errors can compound over time. As might be expected given the water flow results, sediment flow predictions also had a 90-100% average absolute error (depending on if possible outliers were removed) and the Nash Sutcliffe coefficient was around 0, indicating that the model is no better at prediction that using the raw average. One thing to notice in the chart of measured and modeled sediment flow is how much narrower the range of values is for the modeled values compared to measured values; the extremes of the natural world have been muted toward the mean by the model.

Site 3: Olive Orchard Experiment in Cordoba, Spain

Spanish olive model results are described in Figure 10, Figure 11, Figure 12, and Figure 13. Like the DPR trials, results are visually acceptable with the modeled results somewhat tracking measured values. But

when the statistics are investigated, average percent error is over 100% and validated Nash Sutcliffe coefficients for both water and sediment flows are less than zero. .

Conclusions

The integrated RZWQM-Sed model developed in this study works best on field sized areas over a time period ranging from a single runoff event to an entire growing season. Modeled water runoff is highly sensitive to the residual and saturated water content of the soil along with the Brooks-Corey bubbling pressure. Modeled sediment runoff is highly sensitive to the USLE factors and Manning's N.

Calculated flow and sediment loads are often no better than using an average of past measured values. This can be perfectly acceptable for some modeling problems, such as looking at the impact of changing best management practices, so long as the overall change in the calculated average is used for decision making, not individual storm events. End users of the model who work in the pesticide regulatory arena found the predicted water and sediment runoff results from field sized areas to be of acceptable accuracy and better than many models they have utilized. Whether this is a condemnation of field scale agricultural models as a whole or a reflection that Nash-Sutcliffe statistics fail to explain the whole story remains to be seen.

Tracking sorbed chemicals off site is far more accurate than bulk sediment and water flow calculations. One caveat to the performance of the pesticide flow calculations is that RZWQM seems to have a longer tail of out flowing chemical mass compared to measured values. This might be due to governing equations themselves, or may be a result of having to use the average mass present in the first centimeter of soil rather than being able to use a true surface crust concentration. Fine tuning of pesticide parameters, particularly the degradation half lives and degradation modifiers, might fix this issue.

The integrated model generated by this study fills a previously empty niche in the toolbox of models: an agricultural model that tracks offsite sediment and solute flow along with standard farm processes like

vadose zone hydrology, plant growth kinetics, crop management processes, nutrient cycling, and other soil chemical processes. While this collection of attributes makes the integrated model unique in the agricultural modeling world, there is still ample room for improvement.

Tables & Figures

Table 4: DAKOTA optimization parameter values

DAKOTA parameter	Value
multipoint parameterized binary	2
crossover rate	0.8
mutation scale	0.1
shrinkage percentage	0.9
convergence percent change	0.05

Table 5: GLEAMS parameters of interest

Parameter	Description	Units	Min Val	Max Val
SSCLY	Specific surface area for clay particles Suggested values: 20.0 for kaolinite, 800.0 for montmorillonite	m^2/g	20	800
KSOIL	Soil erodibility factor for the slop segment just above start of model	ton/ac or t.ha.h/ha.MJ.mm	0.001	1
CFACT	Soil loss ratio for overland flow profile segment	unitless	0	1
PFACT	Contouring factor for overland flow profile segment	unitless	0.01	1
NFACT	Mannings 'n' for overland flow profile segment.	unitless	0.01	0.14

Table 6: RZWQM parameters of interest

Parameter	Description	Units	Min Val	Max Val
ct	Second intercept on K(h) curve	unitless	0	10000
eps	Exponent for K(h) curve	unitless	2	3
hbk	Bubbling pressure K(h) curve	cm	0	100
hbo	Bubbling pressure	cm	0	100
ksat	Saturated hydraulic conductivity	cm/hr	0	3
lamda	Pore size distribution index	unitless	0	1
latk	Lateral saturated hydraulic conductivity	cm/hr	0	3
swc	Soil water content	cm^3/cm^3	0	0.5
wfca	Field capacity (1/3 bar)	cm^3/cm^3	0	1
wfcb	Field capacity (1/10 bar)	cm^3/cm^3	0	1
wr	Residual water content	cm^3/cm^3	0	1
ws	Saturation water content	cm^3/cm^3	0	1
wwp	Wilting point (15 bar)	cm^3/cm^3	0	1

Table 7: GLEAMS Sobol statistics

Parameter	First_Order	First_Order_Conf	Total_Order	Total_Order_Conf
nfact	0.085	0.028	0.447	0.060
irrig	0.168	0.030	0.378	0.060
cfact	0.097	0.024	0.309	0.075
pfact	0.078	0.022	0.290	0.054
ksoil	0.081	0.022	0.260	0.052
sscly	0.000	0.000	0.000	0.000

Parameter_1	Parameter_2	Second_Order	Second_Order_Conf
nfact	irrig	0.066	0.054
ksoil	nfact	0.058	0.041
cfact	nfact	0.055	0.051
pfact	nfact	0.055	0.043
ksoil	irrig	0.027	0.035
cfact	irrig	0.021	0.046
pfact	irrig	0.018	0.031
cfact	pfact	0.010	0.045
ksoil	pfact	0.007	0.032
ksoil	cfact	0.004	0.035
sscly	ksoil	0.000	0.000
sscly	irrig	0.000	0.000
sscly	cfact	0.000	0.000
sscly	pfact	0.000	0.000
sscly	nfact	0.000	0.000

Notes: Important parameters have a total order > 0.05.
Dominant parameters have a total order > 0.8

Table 8: RZWQM Sobol statistics

Parameter	First_Order	First_Order_Conf	Total_Order	Total_Order_Conf
hbk	0.234059	0.109777	0.719802	0.112246
ws	0.011102	0.061378	0.533612	0.120416
wr	0.020575	0.080453	0.499335	0.117461
ksat	0.035343	0.056374	0.298807	0.103809
hbo	0.001407	0.048829	0.244637	0.09506
lamda	-0.003552	0.054526	0.128847	0.071948
eps	-0.000158	0.033789	0.052119	0.04378
swc	-0.00109	0.002298	0.001158	0.002249

Parameter_1	Parameter_2	Second_Order	Second_Order_Conf
wr	ws	0.099117	0.090781
wr	hbk	0.075746	0.133983
ws	hbk	0.06378	0.103722
hbo	hbk	0.058436	0.095638
ksat	hbk	0.057246	0.087492
lamda	hbk	0.024324	0.068347
ksat	wr	0.012503	0.093768
wr	swc	-0.001699	0.0764
lamda	ksat	-0.004796	0.061313
hbo	wr	-0.004989	0.072704
lamda	swc	-0.005242	0.059208
lamda	eps	-0.005674	0.061776
ksat	ws	-0.005935	0.086711
hbo	lamda	-0.007209	0.065072
eps	ksat	-0.009602	0.044758
eps	wr	-0.009635	0.045143
hbo	eps	-0.010087	0.064041
hbo	ksat	-0.010599	0.06422
ksat	swc	-0.010848	0.081699
lamda	wr	-0.019166	0.062772
eps	ws	-0.021486	0.063793
eps	swc	-0.023055	0.037464
hbo	swc	-0.023069	0.056902
lamda	ws	-0.033471	0.0629
hbo	ws	-0.035141	0.065342
eps	hbk	-0.035863	0.066637
ws	swc	-0.043252	0.066468
hbk	swc	-0.099468	0.161718

Figure 2: RZWQM OAT & Sobol plots

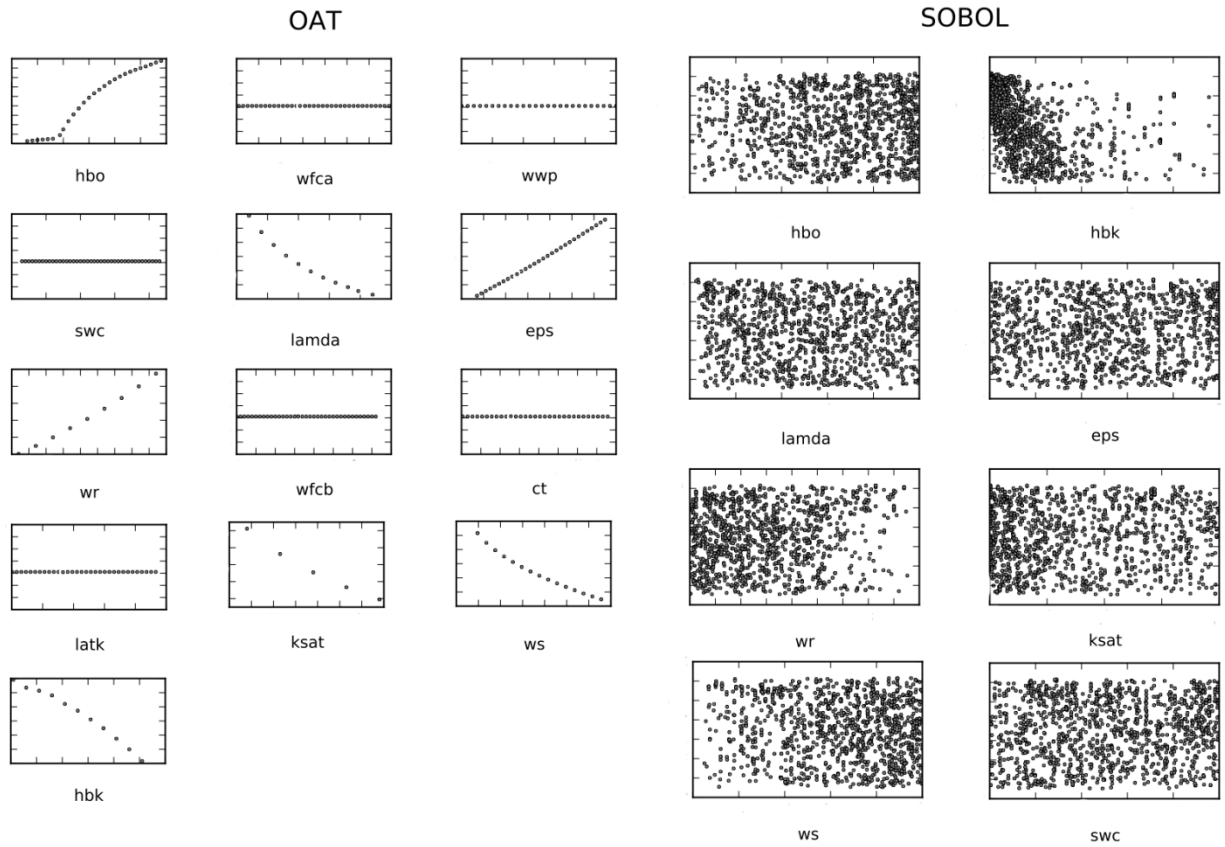


Figure 3: GLEAMS OAT & Sobol plots

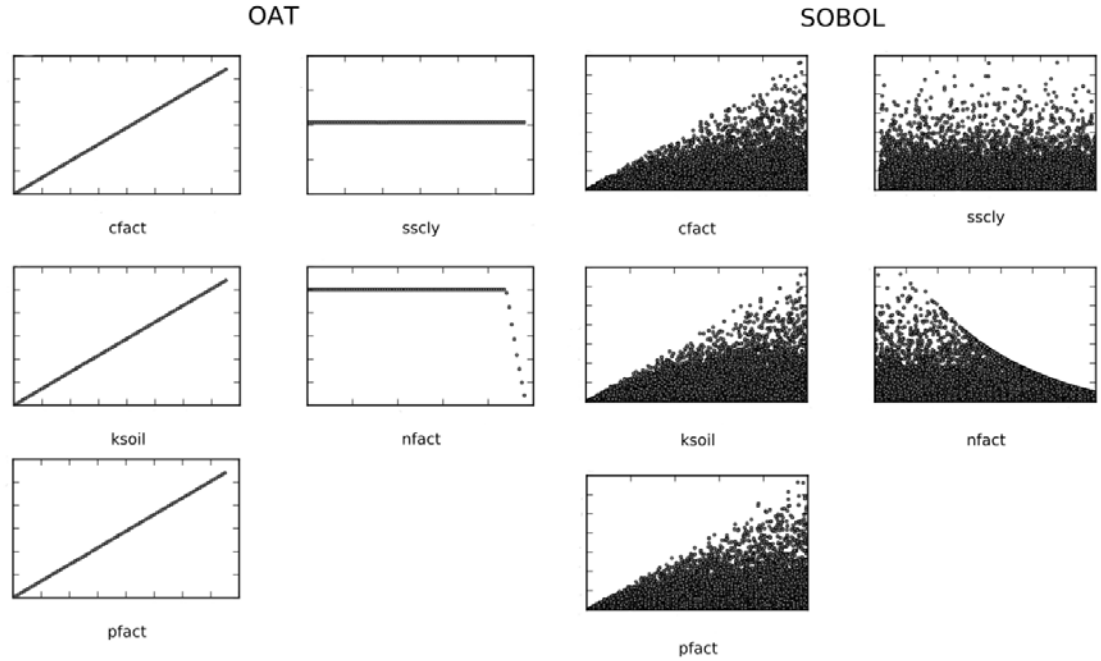


Figure 4: Treynor calibrated flow

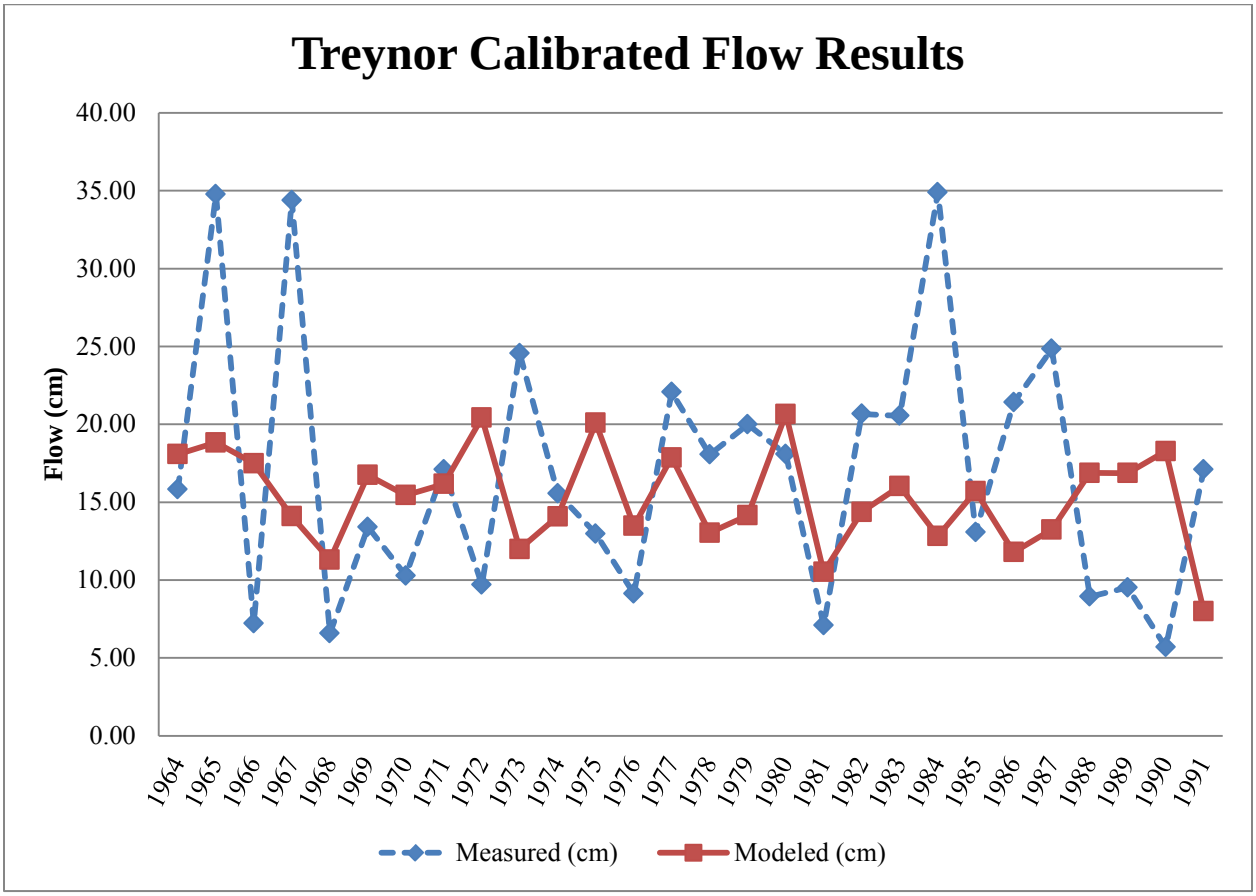


Figure 5: Treynor calibrated sediment

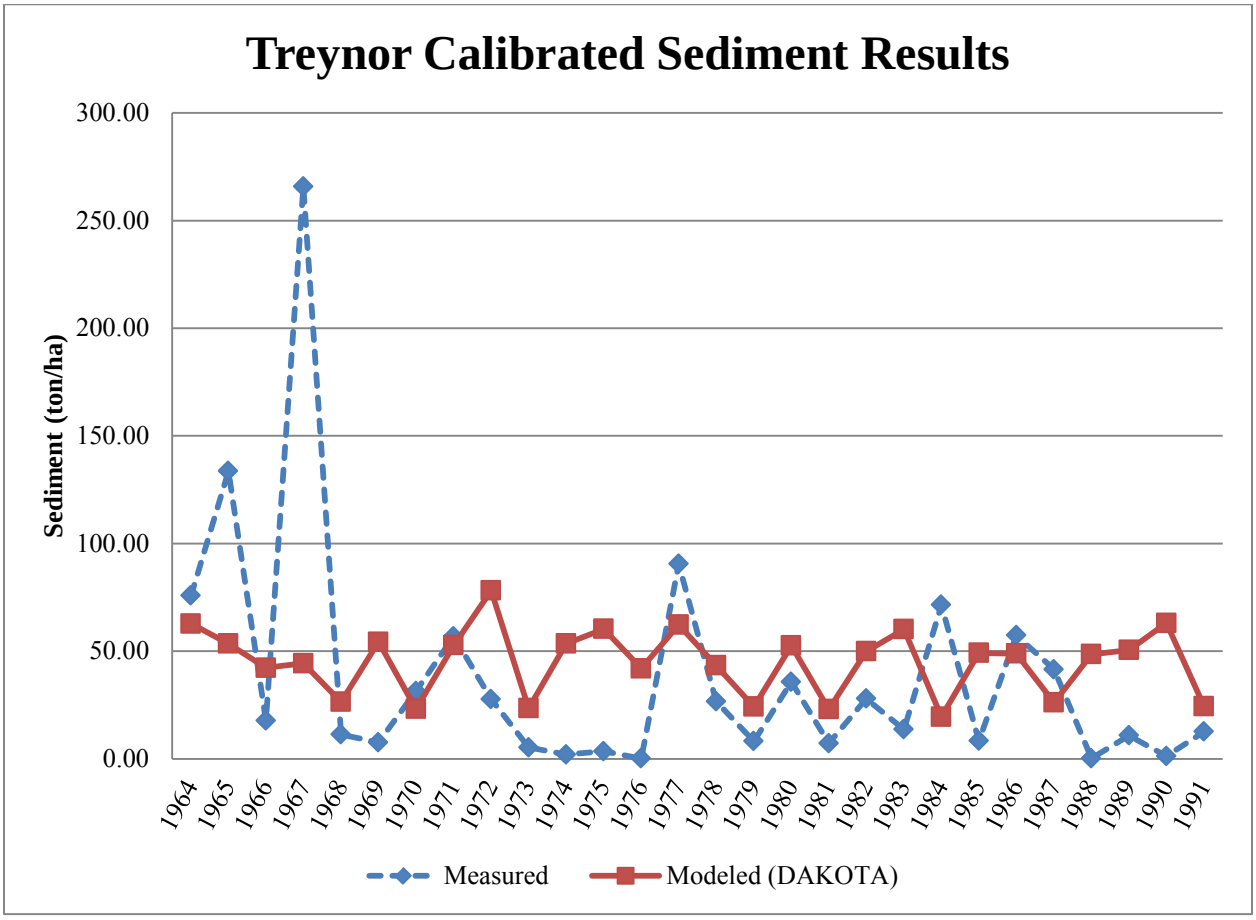


Figure 6: DPR flow

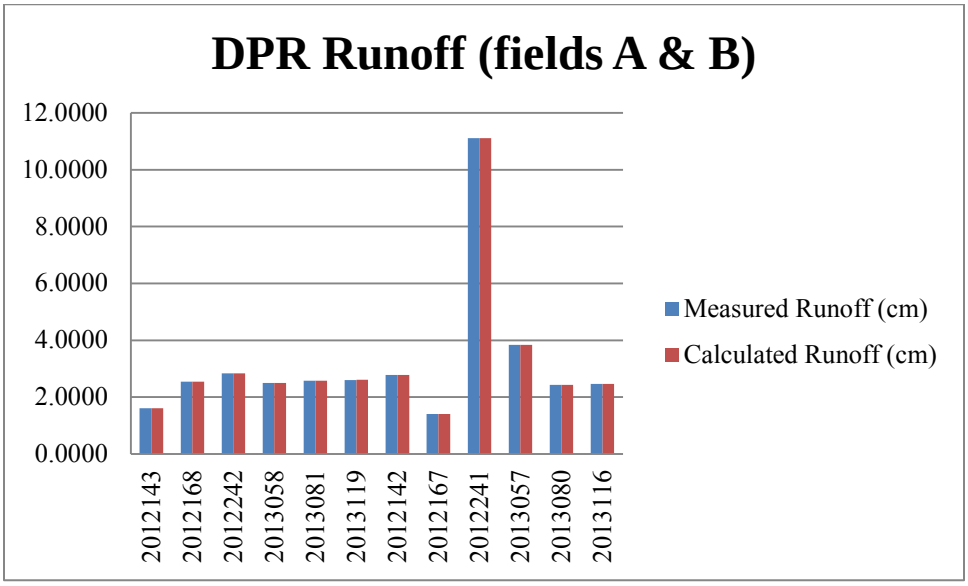


Figure 7: DPR sediment

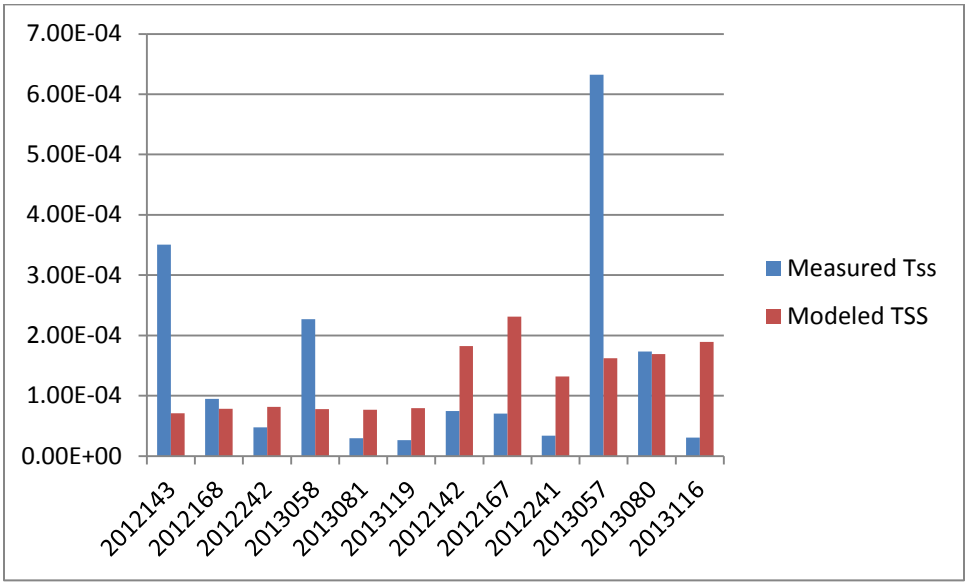


Table 9: DPR flow & sediment results

Julian Day	Field	Measured Runoff (cm)	Calculated Runoff (cm)	%err	Measured Tss (cm^3/cm^3)	Optimized TSS (cm^3/cm^3)	%err
2012143	A	1.61	1.61	0.03	3.51E-04	7.13E-05	79.68
2012168	A	2.54	2.54	0.01	9.48E-05	7.87E-05	16.97
2012242	A	2.83	2.84	0.13	4.78E-05	8.16E-05	70.75
2013058	A	2.5	2.5	0	2.27E-04	7.80E-05	65.65
2013081	A	2.57	2.57	0.01	2.95E-05	7.67E-05	159.78
2013119	A	2.6	2.61	0.23	2.65E-05	7.95E-05	200.23
2012142	B	2.77	2.77	0.02	7.50E-05	1.82E-04	143.22
2012167	B	1.41	1.41	0.02	7.06E-05	2.31E-04	227.59
2012241	B	11.11	11.12	0.05	3.41E-05	1.32E-04	287.91
2013057	B	3.83	3.84	0.13	6.32E-04	1.62E-04	74.34
2013080	B	2.43	2.43	0.03	1.73E-04	1.69E-04	2.32
2013116	B	2.46	2.46	0.02	3.05E-05	1.89E-04	520.60

Table 10: Treynor water flow results

Year	Measured (cm)	Modeled (cm)
1964	15.82	18.09
1965	34.77	18.84
1966	7.21	17.50
1967	34.39	14.10
1968	6.58	11.30
1969	13.41	16.75
1970	10.29	15.45
1971	17.09	16.17
1972	9.70	20.42
1973	24.56	11.99
1974	15.57	14.09
1975	12.98	20.10
1976	9.12	13.48
1977	22.07	17.87
1978	18.06	13.04
1979	19.99	14.16
1980	18.08	20.66
1981	7.09	10.52
1982	20.68	14.38
1983	20.55	16.02
1984	34.90	12.82
1985	13.08	15.71
1986	21.41	11.79
1987	24.84	13.24
1988	8.94	16.88
1989	9.53	16.87
1990	5.69	18.28
1991	17.09	8.01
Avg	16.91	
NS	-0.27	

Table 11: Treynor water flow results w/o outliers

Year	Measured (cm)	Modeled (cm)
1964	15.82	18.09
1965	34.77	18.84
1966	7.21	17.50
1967	34.39	14.10
1968	6.58	11.30
1969	13.41	16.75
1970	10.29	15.45
1971	17.09	16.17
1972	9.70	20.42
1973	24.56	11.99
1974	15.57	14.09
1975	12.98	20.10
1976	9.12	13.48
1977	22.07	17.87
1978	18.06	13.04
1979	19.99	14.16
1980	18.08	20.66
1981	7.09	10.52
1982	20.68	14.38
1983	20.55	16.02
1985	13.08	15.71
1986	21.41	11.79
1987	24.84	13.24
1988	8.94	16.88
1989	9.53	16.87
1990	5.69	18.28
1991	17.09	8.01
Avg	14.78	
NS	-0.51	

Table 12: Treynor sediment flow statistics

Year	Measured	Modeled (DAKOTA)	abs(%err) DAKOTA
1964	75.77	62.77	17.16
1965	133.63	53.55	59.93
1966	17.73	42.26	138.31
1967	265.78	44.34	83.32
1968	11.28	26.43	134.36
1969	7.64	54.33	610.73
1970	31.47	23.19	26.32
1971	56.87	52.74	7.27
1972	27.71	78.16	182.10
1973	5.27	23.53	346.60
1974	2.02	53.48	2550.80
1975	3.52	60.33	1614.12
1976	0.18	41.98	23311.30
1977	90.54	62.32	31.18
1978	26.65	43.37	62.73
1979	8.20	24.23	195.33
1980	35.76	52.64	47.23
1981	7.20	23.08	220.76
1982	27.93	49.91	78.70
1983	13.70	60.20	339.50
1984	71.47	19.52	72.68
1985	8.32	49.23	491.99
1986	57.37	48.92	14.72
1987	41.52	26.19	36.93
1988	0.22	48.62	21590.83
1989	10.87	50.50	364.52
1990	1.26	63.08	4924.67
1991	12.62	24.35	92.93
Avg	37.59		2058.82
NS		0.032	

Table 13: Treynor sediment flow statistics w/o outliers

Year	Measured	Modeled (DAKOTA)	abs(%err) DAKOTA
1964	75.77	62.77	17.16
1966	17.73	42.26	138.31
1968	11.28	26.43	134.36
1969	7.64	54.33	610.73
1970	31.47	23.19	26.32
1971	56.87	52.74	7.27
1972	27.71	78.16	182.10
1973	5.27	23.53	346.60
1974	2.02	53.48	2550.80
1975	3.52	60.33	1614.12
1976	0.18	41.98	23311.30
1977	90.54	62.32	31.18
1978	26.65	43.37	62.73
1979	8.20	24.23	195.33
1980	35.76	52.64	47.23
1981	7.20	23.08	220.76
1982	27.93	49.91	78.70
1983	13.70	60.20	339.50
1984	71.47	19.52	72.68
1985	8.32	49.23	491.99
1986	57.37	48.92	14.72
1987	41.52	26.19	36.93
1988	0.22	48.62	21590.83
1989	10.87	50.50	364.52
1990	1.26	63.08	4924.67
1991	12.62	24.35	92.93
Avg	25.12		2211.68
NS		-0.999	

Table 14: DPR sediment absolute error statistics

Julian Day	Field	Measured Tss	Modeled TSS	abs(%err)
2012143	A	0.000350826	7.12932E-05	79.67846373
2012168	A	9.48229E-05	7.87302E-05	16.97134102
2012242	A	4.78121E-05	8.16403E-05	70.75242226
2013058	A	0.000227028	7.79767E-05	65.65326828
2013081	A	2.95376E-05	7.67339E-05	159.7842331
2013119	A	2.64741E-05	7.94822E-05	200.2258184
2012142	B	7.49937E-05	0.000182399	143.218849
2012167	B	7.06289E-05	0.000231373	227.5899654
2012241	B	3.40528E-05	0.000132094	287.9093728
2013057	B	0.000632486	0.000162297	74.33977836
2013080	B	0.000173201	0.000169188	2.317131572
2013116	B	3.04735E-05	0.000189119	520.6027485
	Avg	0.000149361		154.0869494
	NS	-0.10356079		

Table 15: DPR sediment absolute error statistics w/o outlier

Julian Day	Field	Measured Tss	Modeled TSS	abs(%err)
2012143	A	0.000350826	7.12932E-05	79.67846373
2012168	A	9.48229E-05	7.87302E-05	16.97134102
2012242	A	4.78121E-05	8.16403E-05	70.75242226
2013058	A	0.000227028	7.79767E-05	65.65326828
2013081	A	2.95376E-05	7.67339E-05	159.7842331
2013119	A	2.64741E-05	7.94822E-05	200.2258184
2012142	B	7.49937E-05	0.000182399	143.218849
2012167	B	7.06289E-05	0.000231373	227.5899654
2012241	B	3.40528E-05	0.000132094	287.9093728
2013080	B	0.000173201	0.000169188	2.317131572
2013116	B	3.04735E-05	0.000189119	520.6027485
	Avg	0.000105441		161.3366922
	NS	-0.659022847		

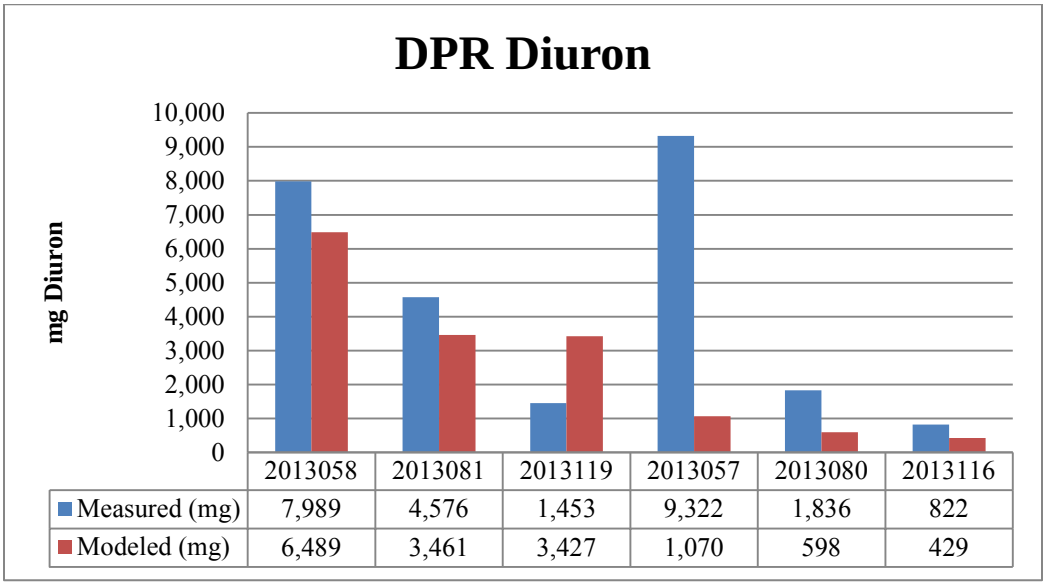
Table 16: DPR Diruron statistics

Date	Field	Measured (mg)	Modeled (mg)	abs(%err)
2013058	A	7,989	6,489	18.78
2013081	A	4,576	3,461	24.37
2013119	A	1,453	3,427	135.81
2013057	B	9,322	1,070	88.52
2013080	B	1,836	598	67.43
2013116	B	822	429	47.84
	Avg	4,333		63.79
	NS	-0.18		

Table 17: DPR Chlorpyfios statistics

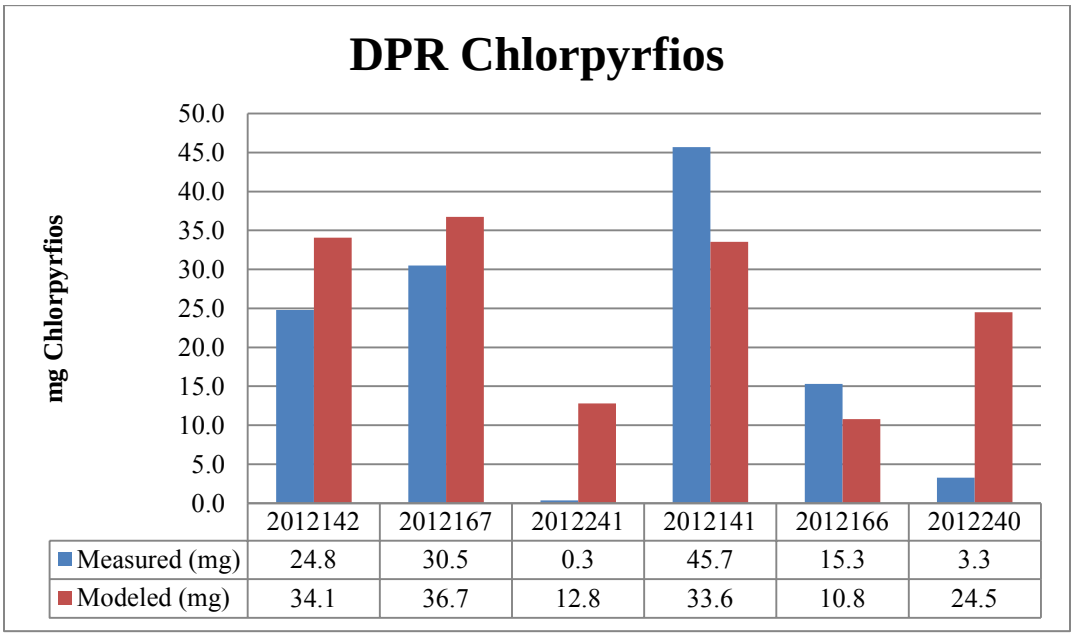
Date	Field	Measured (mg)	Modeled (mg)	abs(%err)
2012142	A	24.8	34.1	37.33
2012167	A	30.5	36.7	20.52
2012241	A	0.3	12.8	3560.57
2012141	B	45.7	33.6	26.59
2012166	B	15.3	10.8	29.46
2012240	B	3.3	24.5	648.12
	Avg	19.99		720.43
	NS	0.39		

Figure 8: DPR Diuron results



	2013058	2013081	2013119	2013057	2013080	2013116
Measured (mg)	7,989	4,576	1,453	9,322	1,836	822
Modeled (mg)	6,489	3,461	3,427	1,070	598	429

Figure 9: DPR Chlorpyrfios results



	2012142	2012167	2012241	2012141	2012166	2012240
Measured (mg)	24.8	30.5	0.3	45.7	15.3	3.3
Modeled (mg)	34.1	36.7	12.8	33.6	10.8	24.5

Figure 10: Olive runoff calibration (NS = 0.67)

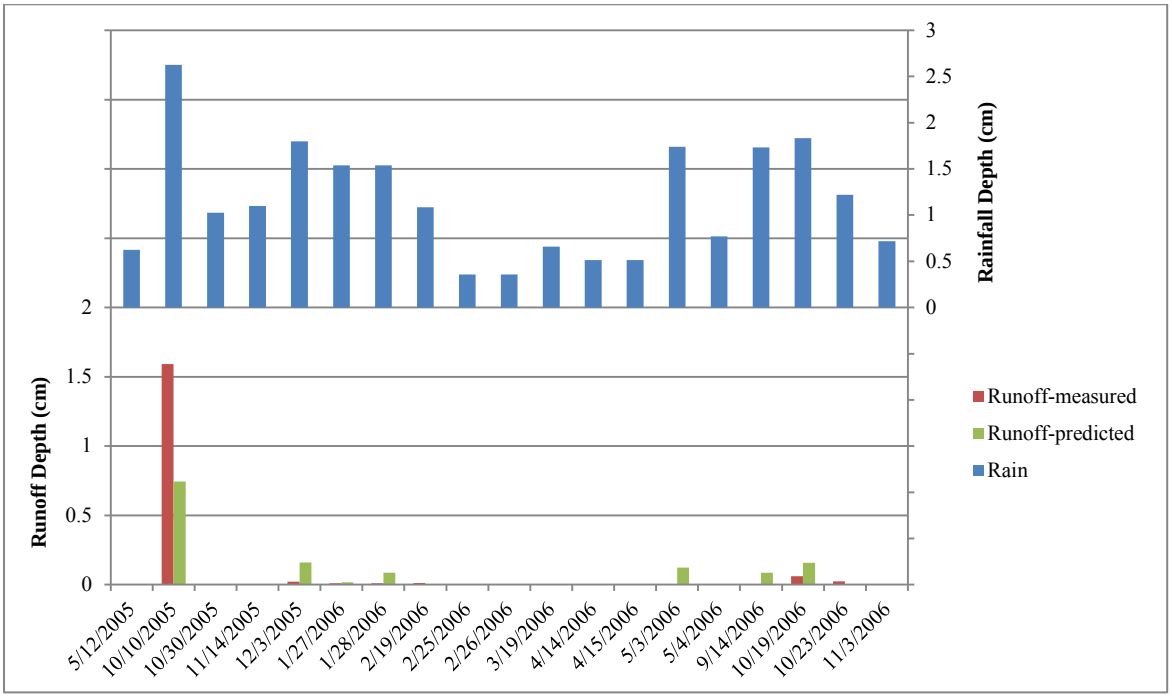


Figure 11: Olive runoff validation (NS = -0.49)

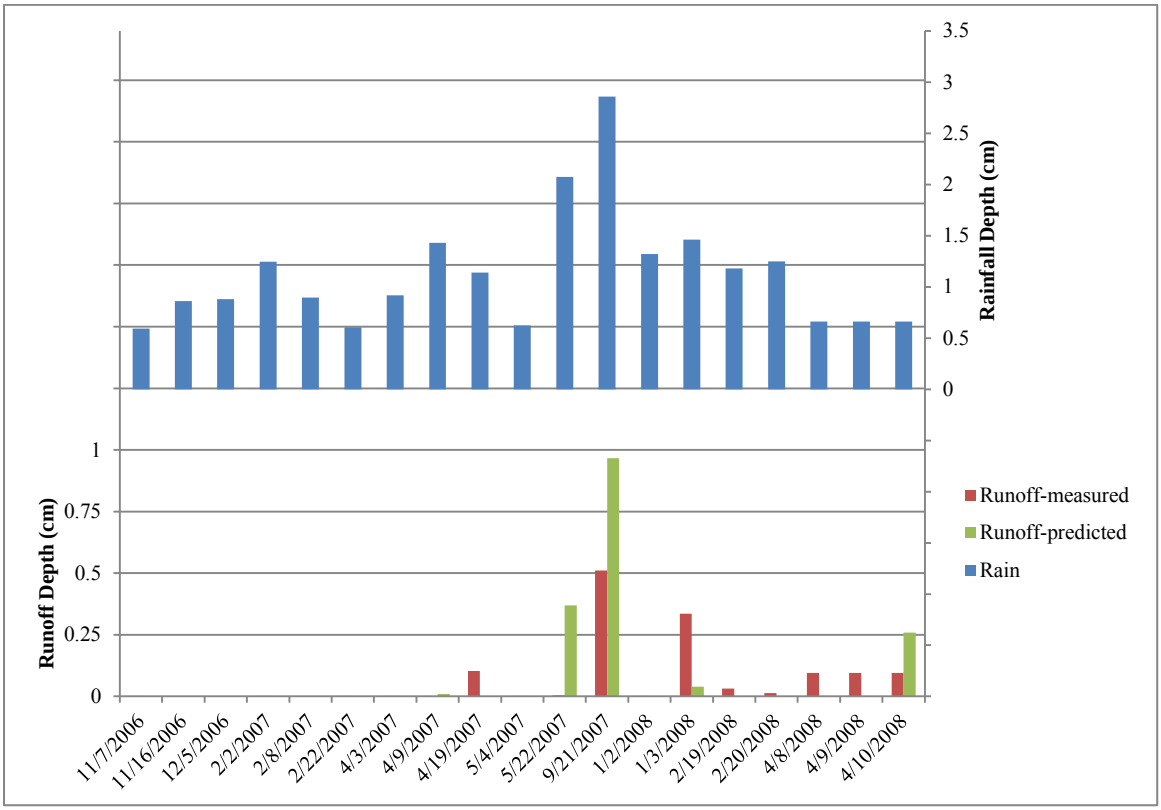


Figure 12: Olive sediment calibration (NS = 0.81)

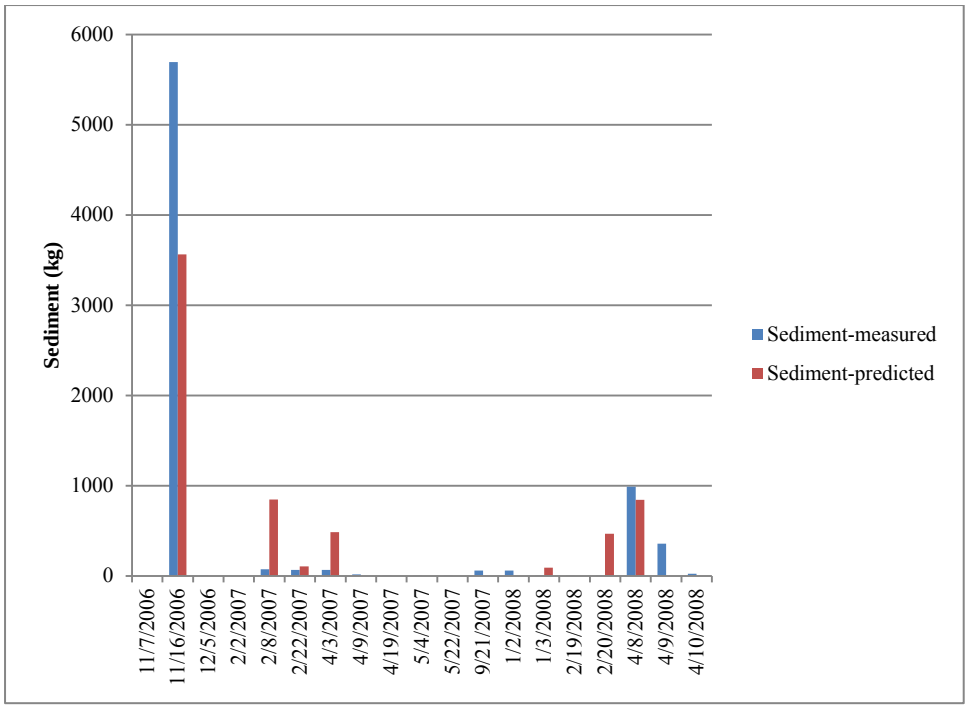


Figure 13: Olive sediment validation (NS = -1.07)

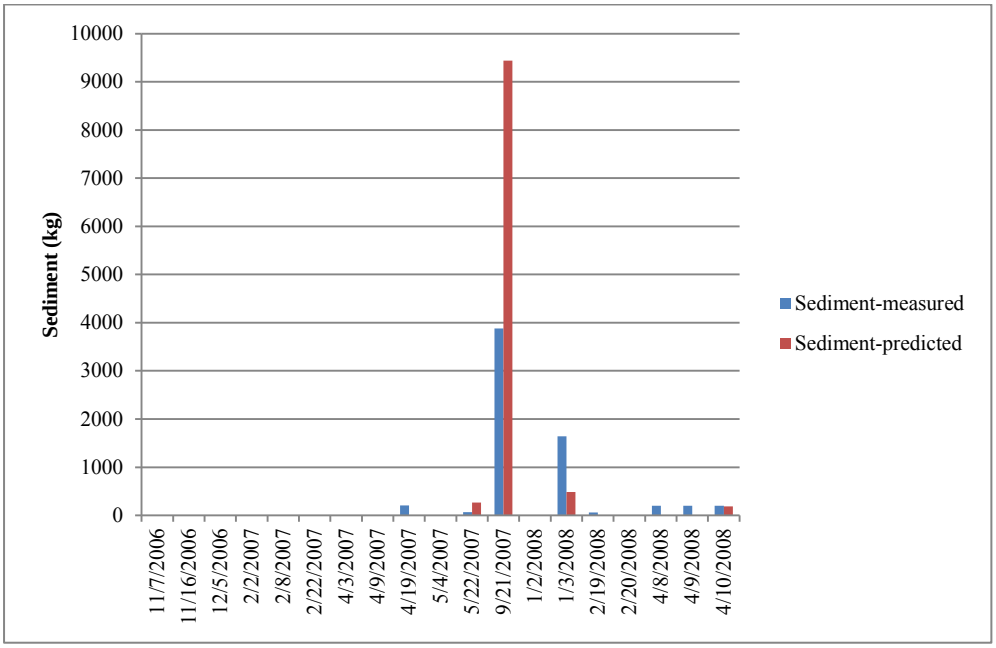
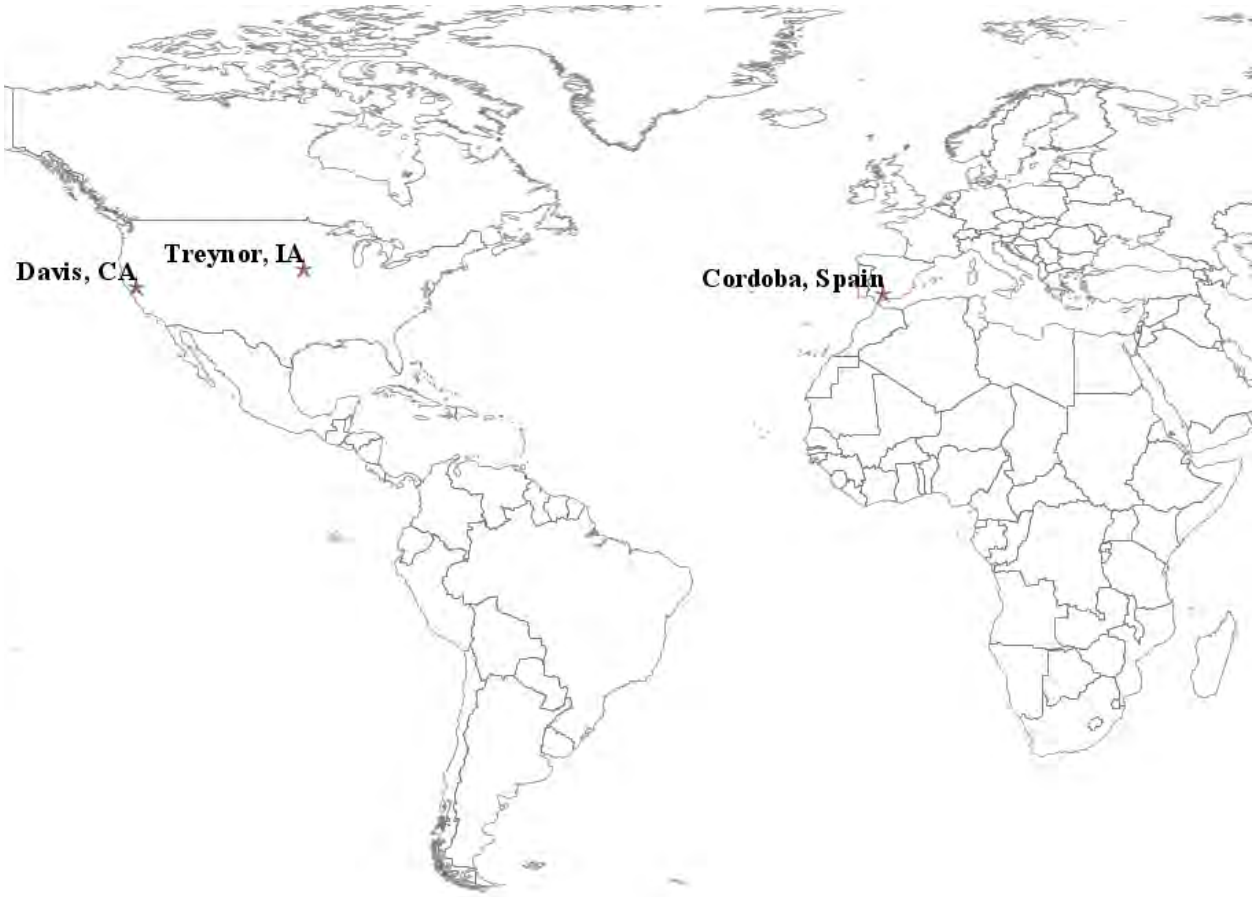


Figure 14 Study Locations



References

1. Wischmeier, W. Use and Misuse of Universal Soil Loss Equation. *J. Soil Water Conserv.* **31,** 5–9 (1976).
2. Renard, K. G., Foster, G. R., Weesies, G. A. & Porter, J. P. RUSLE: Revised universal soil loss equation. *J. Soil Water Conserv.* **46,** 30–33 (1991).
3. M Littleboy, D. S. Impact of soil erosion on production in cropping systems .I. Development and validation of a simulation model. *Aust. J. Soil Res. - AUST J SOIL RES* **30,** (1992).
4. United States. Science and Education Administration & Knisel, W. G. *CREAMS : a field scale model for Chemicals, Runoff, and Erosion from Agricultural Management Systems*. ([Washington] : Dept. of Agriculture, Science and Education Administration, 1980). at <http://archive.org/details/creamsfieldscale26unit>
5. Leonard, R., Knisel, W. & Still, D. Gleams - Groundwater Loading Effects of Agricultural Management-Systems. *Trans. Asae* **30,** 1403–1418 (1987).
6. Young, R. A. (Robert A. & United States. Agricultural Research Service. *AGNPS, Agricultural Non-Point-Source Pollution Model : a watershed analysis tool*. ([Washington, D.C.] : U.S. Dept. of Agriculture, Agricultural Research Service, 1987). at <http://archive.org/details/agnpsagricultura35youn>
7. Vertessy, R. A. *et al.* New software to aid water quality management in the catchments and waterways of the south-east Queensland region. in *Proceedings of the 3rd Australian Stream Management Conference, Brisbane* (2001). at <http://www.researchgate.net/publication/252531875_New_software_to_aid_water_quality_management_in_the_catchments_and_waterways_of_the_south-east_Queensland_region/file/3deec529e9de487be8.pdf>

8. Viney, N. R. & Sivapalan, M. A conceptual model of sediment transport: application to the Avon River Basin in Western Australia. *Hydrol. Process.* **13,** 727–743 (1999).

9. Arnold, J. G. *SWRRB: a basin scale simulation model for soil and water resources management*. (Texas A & M University Press, 1990).

10. Beasley, D., Huggins, L. & Monke, E. Answers - a Model for Watershed Planning. *Trans. Asae* **23,** 938–944 (1980).

11. Yu, B., Rose, C., Ciesiolka, C. A. A., Coughlan, K. J. & Fentie, B. Towards a framework for runoff and soil loss prediction using GUEST technology. *Aust. J. Soil Res.* **35,** 1191–1212 (1997).

12. Bicknell, B. R., Imhoff, J. C., Kittle, J. L. J., Donigian, A. S. J. & Johanson, R. C. *Hydrological Simulation Program--Fortran, User's manual for version 11*. (U.S. Environmental Protection Agency, National Exposure Research Laboratory, 1997).

13. Takken, I. *et al.* Spatial evaluation of a physically-based distributed erosion model (LISEM). *CATENA* **37,** 431–447 (1999).

14. Laflen, J. M., Lane, L. J. & Foster, G. R. WEPP: A new generation of erosion prediction technology. *J. Soil Water Conserv.* **46,** 34–38 (1991).

15. Govers, G. Empirical relationships for the transport capacity of overland flow. 45–63 (1990).

16. Ahuja, L., Rojas, K. W. & Hanson, J. D. *Root Zone Water Quality Model: Modelling Management Effects on Water Quality and Crop Production*. (Water Resources Publication, 2000).

17. Heber Green, W. & Ampt, G. A. Studies on Soil Phyics. *J. Agric. Sci.* **4,** 1–24 (1911).

18. Bouwer, H. Calculating Infiltration into Non-Uniform Soil with Green and Ampt Approach. *Agric. Eng.* **50,** 610–& (1969).

19. Morel-Seytoux, H. J. & Khanji, J. Derivation of an equation of infiltration. *Water Resour. Res.* **10,** 795–800 (1974).

20. Brakensiek, D. & Onstad, C. Parameter-Estimation of Green and Ampt Infiltration Equation. *Water Resour. Res.* **13,** 1009–1012 (1977).

21. Brooks, R. J. & Corey, A. T. Hydraulic properties of porous media. *Hydrol. Pap.* **3,** (1964).

22. W. G. Knisel & K. R. Douglas-Mankin. CREAMS/GLEAMS: Model Use, Calibration, and Validation. *Trans. ASABE* **55,** 1291–1302 (2012).

23. Taguas, E. V., Moral, C., Ayuso, J. L., Pérez, R. & Gómez, J. A. Modeling the spatial distribution of water erosion within a Spanish olive orchard microcatchment using the SEDD model. *Geomorphology* **133,** 47–56 (2011).

24. Cryer, S. A. & Havens, P. L. Regional sensitivity analysis using a fractional factorial method for the USDA model GLEAMS. *Environ. Model. Softw.* **14,** 613–624 (1999).

25. Persicani, D. Pesticide leaching into field soils: sensitivity analysis of four mathematical models. *Ecol. Model.* **84,** 265–280 (1996).

26. S. Wedwick, B. Lakhani, J. Stone, P. Waller & J. Artiola. DEVELOPMENT AND SENSITIVITY ANALYSIS OF THE GLEAMS–IR MODEL. *Trans. ASAE* **44,** (2001).

27. Ahmed, I., Rudra, R., McKague, K., Gharabaghi, B. & Ogilvie, J. Evaluation of the Root Zone Water Quality Model (RZWQM) for Southern Ontario: Part I. Sensitivity Analysis, Calibration, and Validation. *Water Qual. Res. J. Can.* **42,** 202–218 (2007).

28. Morris, M. Factorial Sampling Plans for Preliminary Computational Experiments. *Technometrics* **33,** 161–174 (1991).

29. Sobol, I. M. Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. *Math. Comput. Simul.* **55,** 271–280 (2001).

30. Sobol', I. . On the distribution of points in a cube and the approximate evaluation of integrals. *USSR Comput. Math. Math. Phys.* **7,** 86–112 (1967).

31. Adams, B.M., Bohnhoff, W.J., Dalbey, K.R., Eddy, J.P., Eldred, M.S., Gay, D.M., Haskell, K., Hough, P.D., and Swiler, L.P. *DAKOTA, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 5.0 User's Manual*. (2013).

32. Eddy, J. & Lewis, K. Effective Generation of Pareto Sets Using Genetic Programming. (2001). at <http://does.eng.buffalo.edu/index.php?option=com_jresearch&view=publication&task=show&id=59&Itemid=53>

Appendix F: Poster Presented at the 2014 ASA, CSSA, and SSSA Annual Meeting in Long Beach, CA (poster.ppt)

UCDAVIS
UNIVERSITY OF CALIFORNIA

Integrating GLEAMS sedimentation into RZWQM, sensitivity analysis, and evaluation

Christopher DeMars, LAWR Hydrology, UC Davis: chdemars@ucdavis.edu

dpr

Introduction

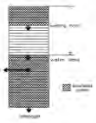
Sediment runoff, particularly chemically sorbed sediment from agricultural activities, is an acute environmental problem. There is currently a lack of agricultural models that support chemically sorbed sediment flow.

Objectives of this study:

- Integrate the sediment and surface flow components of Groundwater Loading Effects of Agricultural Management Systems (GLEAMS)[1] model into the Root Water Quality Model (RZWQM)[2]
- Perform a sensitivity analysis
- Assess the model's accuracy by calibrating and validating it against multiple real world datasets

RZWQM

- Vertical one dimensional
- 12 user defined soil layers
- Internal computation on 1cm thick soil layers
- Daily time step: plant growth, soil chemistry, nutrients, pesticides, site management, evapotranspiration
- Sub-hourly time step: heat transport, water balance, solute transport, snowpack dynamics, chemical uptake



GLEAMS

- Extension of the CREAMS[3] model
- Developed during the 1980s at the USDA-ARS
- Erosion component remained relatively unchanged compared to CREAMS
- Sediment movement: horizontal 1D set of linked reaches
- Sediment loss of each reach governed by a modified Universal Soil Loss Equation (USLE)[4].

Methodology

- RZWQM and GLEAMS coded in Fortran
- Compiled for this study on Windows 7 using Intel Fortran and Microsoft Visual Studio
- Two phase sensitivity analysis: One-At-A-Time (OAT) Morris[5] followed by a Sobol[6] analysis.
- Design Analysis Kit for Optimization and Terascale Applications (DAKOTA)[7] used for automated calibration in a two stage process: runoff volume was first calibrated, then sediment mass.
- Optimization was completed using a global, gradient free, genetic algorithm. [8]

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Funding Source

California Department of Pesticide Regulation: contract #11-C0091

Site Locations Studied

Three field sites were chosen spanning time, slope, and crop types.

- multi-year field scale alfalfa trial: *Davis, CA*
- multi-decade watershed scale corn trial: *Treynor, IA*
- multi-year olive orchard trial: *Cordoba, Spain*

Davis, CA alfalfa

- Collected experimental data from two alfalfa fields (0.27ha each, 15.8m wide by 198.12m long) in Davis, California
- Soil: Yolo silty loam (35/40/25 Sand/Silt/Clay), 0.14% slope
- Seven 2012 flood irrigation events (~3cm runoff/event), four 2013 events.
- Input and output flow measurements taken every 2min, sediment measurements taken approximately every 30min.

Treynor, IA Corn

- Data from the Deep Loess Research Station located near Treynor, Iowa.
- Silt-loam soils are classified as Typic Haplorthents and Cumulic Hapludolls; fine silty, mixed mesics; have moderate to moderately rapid permeability.
- Average slope 8 to 9 percent; maximum slope of 18 percent.
- Watershed area is 30.4ha
- Continuous corn between 1964 and 1996
- No irrigation was performed; precipitation left unmodified from the measured values.
- Model run over sub-daily time steps.
- Calibration and validation done using yearly summations to match available data.

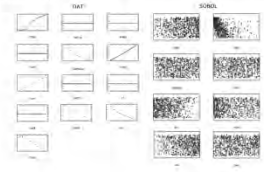
Cordoba Spain olive

- Data obtained from the paper by Tagnas et al[9]
- Study site is an olive planted microcatchment 6.1ha in size located in Province of Cordoba, Spain (37.4°N, 4.8°W)
- Mean elevation of 239m and mean slope of 15%.
- Soil is Cambisol, a loamy sand soil with an organic matter content of 1.6% and bulk density of 1.61g/cm^3.
- Olive trees were planted in 1999 with 7m of space between trees.
- Rainfall, runoff, and sediment loads recorded from May 2005 to February 2008.
- No irrigation was applied, all water input was from rainfall.

Sensitivity Analysis Results

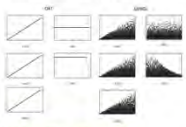
RZWQM Sensitive Variables

- Greatest influence: residual water content (wr), saturated water content (ws), Brooks-Corey bubbling pressure (hbk)
- Lesser influence: hydraulic conductivity (ksat) and the non-Brooks-Corey bubbling pressure (hbo)
- None of the total order results show a dominant influence (total order > 0.8)



GLEAMS Sensitive Variables

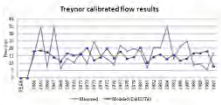
- USLE parameters (cfact, pfact, ksoil) have expected positive linear response
- Manning's N (nfact): no influence until threshold is reached, then quick negative response. More influential when modeling unplanted ground

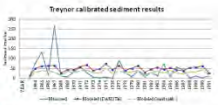


Calibration Results

Treynor, IA corn

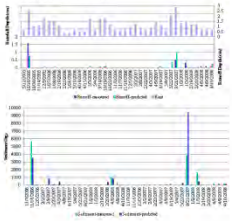
- Predictions of water flow were unimpressive for either the calibrated or validated dataset with an average percent error of ~100% and a Nash Sutcliffe coefficient of ~0.5 to ~0.3 depending on if possible outliers are removed.
- Sediment flow predictions had a 90-100% average absolute error and Nash Sutcliffe coefficient around zero.
- Range of modeled sediment flow values are much narrower compared to measured values





Cordoba Spain olive

- Calculated water & sediment runoff are visually similar to measured results, but
- Average percent error is over 100% and Nash Sutcliffe coefficients for both water and sediment flows are less than zero



Davis, CA alfalfa

- RZWQM doesn't natively support flood irrigation therefore the Davis DPR water runoff was hand calibrated.
- Results: over 100% average percent error and a negative Nash Sutcliffe coefficient; minimal difference in sediment flow from event to event with all flows clustering tight around the mean.
- Pesticide runoff results better than the sediment results with predicted values tracking measured values rather well.
- The 2013057 diuron trial showed an extreme spread between measured and modeled. When removed, the average percent error drops to 59% and the Nash Sutcliffe coefficient becomes a very strong 0.74.
- Chlorpyrifos trials have no obvious outlier and Nash Sutcliffe coefficient of 0.39. Average absolute error is high at 720%, but that drops to 152% with the removal of trial 2012241 which has a 3,560% error.

Conclusions

- RZWQM-GLEAMS works best on field sized areas over a growing season.
- Calculated flow and sediment loads are often no better than using an average of past measured values.
- Tracking sorbed chemicals off site quite accurate
- Results from this model should be interpreted as the likely average of many field trials with the same soil and water input parameters.
- This average sediment loading value can be used to estimate sediment transport off field in order to design sediment traps and other mitigation measures.
- Sediment flow and solute concentration can be used to model various BMPs that modify pesticide application and irrigation timing to minimize solute transport off the field
- Neither RZWQM nor GLEAMS allow for much complexity: simplifies 3D space into a pair of 1D flow lines and limits the number of computation cells to double digits or less

References

1. Leonard, R. Knisel, W. G. (Ed.). D. Osborn (Associate Editor) Effected Agricultural Management Systems. Pub. Ann (Ed.), 643 p. (1993).
2. L. Ma et al. Root Zone Water Quality Model (RZWQM2): Model Use, Calibration, and Validation. Trans. ASABE 55, 1425-1446 (2012).
3. United States. Science and Education Administration. R. Knisel, W.G. CREAMS: a field scale model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. (Washington). Dept. of Agriculture, Science and Education Administration, 1980. at <http://catalog.hathitrust.org/Record/002460486>
4. Wischmeier, W. The and Moment of Universal Soil Loss Equation. J. Soil Water Conserv. 30, 2-8 (1975).
5. Morris, M. Factorial Sampling Plans for Preliminary Computational Experiments. Technometrics 33, 161-174 (1991).
6. Sobol, I. Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. Math. Comput. Simul. 55, 271-280 (2001).
7. Adams, B.M., Bohnhoff, W.J., Dalbey, K.R., Eddy, J.P., Eldred, M.S., Gay, D.M., Haskell, K., Hough, P.D., and Swiler, L.P. DAKOTA, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis. Version 5.2 User's Manual. (2013).
8. Fabiyi, O., Lewis, R. Effective Discretization of Parameter Space in Genetic Algorithm Optimization. (2011). at <http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.225.9165&rep=rep1&type=pdf>
9. Tagnas, F.Z., Mesa, J.C., Arquero, J.L., Pérez, R. & Tolosana, J. A. Modelling the spatial distribution of water erosion within a Spanish olive orchard using the RZWQ model. Geomorphology 188, 87–98 (2013).

Appendix G: References

1. Ahuja, L., Rojas, K. W. & Hanson, J. D. *Root Zone Water Quality Model: Modelling Management Effects on Water Quality and Crop Production*. (Water Resources Publication, 2000).
2. Jha, S. K. & Bombardelli, F. A. Theoretical/numerical model for the transport of non-uniform suspended sediment in open channels. *Adv. Water Resour.* **34,** 577–591 (2011).
3. Laflen, J. M., Lane, L. J. & Foster, G. R. WEPP: A new generation of erosion prediction technology. *J. Soil Water Conserv.* **46,** 34–38 (1991).
4. Yalin, Y. S. An expression for bed-load transportation. *J Hydraul. Div Proc Am Soc Civ. Engs* **89(HY3),** 221–250 (1963).
5. Wischmeier, W. Use and Misuse of Universal Soil Loss Equation. *J. Soil Water Conserv.* **31,** 5–9 (1976).
6. Renard, K. G., Foster, G. R., Weesies, G. A. & Porter, J. P. RUSLE: Revised universal soil loss equation. *J. Soil Water Conserv.* **46,** 30–33 (1991).
7. M Littleboy, D. S. Impact of soil erosion on production in cropping systems .I. Development and validation of a simulation model. *Aust. J. Soil Res. - AUST J SOIL RES* **30,** (1992).
8. United States. Science and Education Administration & Knisel, W. G. *CREAMS : a field scale model for Chemicals, Runoff, and Erosion from Agricultural Management Systems*. ([Washington] : Dept. of Agriculture, Science and Education Administration, 1980). at <http://archive.org/details/creamsfieldscale26unit>
9. Leonard, R., Knisel, W. & Still, D. Gleams - Groundwater Loading Effects of Agricultural Management-Systems. *Trans. Asae* **30,** 1403–1418 (1987).
10. Young, R. A. (Robert A. & United States. Agricultural Research Service. *AGNPS, Agricultural Non-Point-Source Pollution Model : a watershed analysis tool*. ([Washington, D.C.] : U.S. Dept. of Agriculture, Agricultural Research Service, 1987). at <http://archive.org/details/agnpsagricultura35youn>

11. Vertessy, R. A. *et al.* New software to aid water quality management in the catchments and waterways of the south-east Queensland region. in *Proceedings of the 3rd Australian Stream Management Conference, Brisbane* (2001). at <http://www.researchgate.net/publication/252531875_New_software_to_aid_water_quality_management_in_the_catchments_and_waterways_of_the_south-east_Queensland_region/file/3deec529e9de487be8.pdf>
12. Viney, N. R. & Sivapalan, M. A conceptual model of sediment transport: application to the Avon River Basin in Western Australia. *Hydrol. Process.* **13,** 727–743 (1999).
13. Arnold, J. G. *SWRRB: a basin scale simulation model for soil and water resources management*. (Texas A & M University Press, 1990).
14. Beasley, D., Huggins, L. & Monke, E. Answers - a Model for Watershed Planning. *Trans. Asae* **23,** 938–944 (1980).
15. Yu, B., Rose, C., Ciesiolka, C. A. A., Coughlan, K. J. & Fentie, B. Towards a framework for runoff and soil loss prediction using GUEST technology. *Aust. J. Soil Res.* **35,** 1191–1212 (1997).
16. Bicknell, B. R., Imhoff, J. C., Kittle, J. L. J., Donigian, A. S. J. & Johanson, R. C. *Hydrological Simulation Program--Fortran, User's manual for version 11*. (U.S. Environmental Protection Agency, National Exposure Research Laboratory, 1997).
17. Takken, I. *et al.* Spatial evaluation of a physically-based distributed erosion model (LISEM). *CATENA* **37,** 431–447 (1999).
18. Govers, G. Empirical relationships for the transport capacity of overland flow. 45–63 (1990).
19. Heber Green, W. & Ampt, G. A. Studies on Soil Phyics. *J. Agric. Sci.* **4,** 1–24 (1911).
20. Bouwer, H. Calculating Infiltration into Non-Uniform Soil with Green and Ampt Approach. *Agric. Eng.* **50,** 610–& (1969).
21. Morel-Seytoux, H. J. & Khanji, J. Derivation of an equation of infiltration. *Water Resour. Res.* **10,** 795–800 (1974).

22. Brakensiek, D. & Onstad, C. Parameter-Estimation of Green and Ampt Infiltration Equation. *Water Resour. Res.* **13,** 1009–1012 (1977).

23. Brooks, R. J. & Corey, A. T. Hydraulic properties of porous media. *Hydrol. Pap.* **3,** (1964).

24. W. G. Knisel & K. R. Douglas-Mankin. CREAMS/GLEAMS: Model Use, Calibration, and Validation. *Trans. ASABE* **55,** 1291–1302 (2012).

25. Taguas, E. V., Moral, C., Ayuso, J. L., Pérez, R. & Gómez, J. A. Modeling the spatial distribution of water erosion within a Spanish olive orchard microcatchment using the SEDD model. *Geomorphology* **133,** 47–56 (2011).

26. Adams, B.M., Bohnhoff, W.J., Dalbey, K.R., Eddy, J.P., Eldred, M.S., Gay, D.M., Haskell, K., Hough, P.D., and Swiler, L.P. *DAKOTA, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 5.0 User's Manual*. (2013).

27. Eddy, J. & Lewis, K. Effective Generation of Pareto Sets Using Genetic Programming. (2001). at <http://does.eng.buffalo.edu/index.php?option=com_jresearch&view=publication&task=show&id=59&Itemid=53>

28. Cryer, S. A. & Havens, P. L. Regional sensitivity analysis using a fractional factorial method for the USDA model GLEAMS. *Environ. Model. Softw.* **14,** 613–624 (1999).

29. Persicani, D. Pesticide leaching into field soils: sensitivity analysis of four mathematical models. *Ecol. Model.* **84,** 265–280 (1996).

30. S. Wedwick, B. Lakhani, J. Stone, P. Waller & J. Artiola. DEVELOPMENT AND SENSITIVITY ANALYSIS OF THE GLEAMS–IR MODEL. *Trans. ASAE* **44,** (2001).

31. Ahmed, I., Rudra, R., McKague, K., Gharabaghi, B. & Ogilvie, J. Evaluation of the Root Zone Water Quality Model (RZWQM) for Southern Ontario: Part I. Sensitivity Analysis, Calibration, and Validation. *Water Qual. Res. J. Can.* **42,** 202–218 (2007).

32. Morris, M. Factorial Sampling Plans for Preliminary Computational Experiments. *Technometrics* **33,** 161–174 (1991).

33. Sobol, I. M. Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. *Math. Comput. Simul.* **55,** 271–280 (2001).

34. Sobol', I. . On the distribution of points in a cube and the approximate evaluation of integrals. *USSR Comput. Math. Math. Phys.* **7,** 86–112 (1967).